

L Number	Hits	Search Text	DB	Time stamp
1	1	("5767322").PN.	USPAT; US-PGPUB	2002/09/05 18:20
2	34	cumene adj hydroperoxide adj water	USPAT; US-PGPUB	2002/09/05 18:24
3	28	cumene adj hydroperoxide adj mixture	USPAT; US-PGPUB	2002/09/05 18:24
4	8	cumene adj hydroperoxide adj composition	USPAT; US-PGPUB	2002/09/05 18:24
5	35	(cumene adj hydroperoxide adj mixture) or (cumene adj hydroperoxide adj composition)	USPAT; US-PGPUB	2002/09/05 18:25
6	32	((cumene adj hydroperoxide adj mixture) or (cumene adj hydroperoxide adj composition)) and ( water or H2O)	USPAT; US-PGPUB	2002/09/05 18:25

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LOGINID:sssptal204jxv

PASSWORD:

TERMINAL (ENTER 1, 2, 3, OR ?):2

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NEWS 2 Apr 08 "Ask CAS" for self-help around the clock  
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NEWS 6 Apr 22 Records from IP.com available in CAPLUS, HCAPLUS, and ZCAPLUS  
NEWS 7 Apr 22 BIOSIS Gene Names now available in TOXCENTER  
NEWS 8 Apr 22 Federal Research in Progress (FEDRIP) now available  
NEWS 9 Jun 03 New e-mail delivery for search results now available  
NEWS 10 Jun 10 MEDLINE Reload  
NEWS 11 Jun 10 PCTFULL has been reloaded  
NEWS 12 Jul 02 FOREGE no longer contains STANDARDS file segment  
NEWS 13 Jul 22 USAN to be reloaded July 28, 2002;  
saved answer sets no longer valid  
NEWS 14 Jul 29 Enhanced polymer searching in REGISTRY  
NEWS 15 Jul 30 NETFIRST to be removed from STN  
NEWS 16 Aug 08 CANCERLIT reload  
NEWS 17 Aug 08 PHARMAMarketLetter(PHARMAML) - new on STN  
NEWS 18 Aug 08 NTIS has been reloaded and enhanced  
NEWS 19 Aug 19 Aquatic Toxicity Information Retrieval (AQUIRE)  
now available on STN  
NEWS 20 Aug 19 IFIPAT, IFICDB, and IFIUDB have been reloaded  
NEWS 21 Aug 19 The MEDLINE file segment of TOXCENTER has been reloaded  
NEWS 22 Aug 26 Sequence searching in REGISTRY enhanced  
NEWS 23 Sep 03 JAPIO has been reloaded and enhanced  
  
NEWS EXPRESS February 1 CURRENT WINDOWS VERSION IS V6.0d,  
CURRENT MACINTOSH VERSION IS V6.0a(ENG) AND V6.0Ja(JP),  
AND CURRENT DISCOVER FILE IS DATED 05 FEBRUARY 2002  
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FILE 'HOME' ENTERED AT 17:20:54 ON 05 SEP 2002

=> file caplus

COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	0.21	0.21

FILE 'CAPLUS' ENTERED AT 17:21:16 ON 05 SEP 2002  
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FILE COVERS 1907 - 5 Sep 2002 VOL 137 ISS 10  
 FILE LAST UPDATED: 4 Sep 2002 (20020904/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

CAS roles have been modified effective December 16, 2001. Please check your SDI profiles to see if they need to be revised. For information on CAS roles, enter HELP ROLES at an arrow prompt or use the CAS Roles thesaurus (/RL field) in this file.

=> file reg		
COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	0.40	0.61

FILE 'REGISTRY' ENTERED AT 17:21:28 ON 05 SEP 2002  
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STRUCTURE FILE UPDATES: 4 SEP 2002 HIGHEST RN 446821-48-3  
 DICTIONARY FILE UPDATES: 4 SEP 2002 HIGHEST RN 446821-48-3

TSCA INFORMATION NOW CURRENT THROUGH MAY 20, 2002

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Calculated physical property data is now available. See HELP PROPERTIES for more information. See STNote 27, Searching Properties in the CAS Registry File, for complete details:  
<http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf>

=> s cumene hydroperoxide/cn  
 L1 1 CUMENE HYDROPEROXIDE/CN

=> d

L1 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2002 ACS  
 RN 80-15-9 REGISTRY  
 CN Hydroperoxide, 1-methyl-1-phenylethyl (9CI) (CA INDEX NAME)

OTHER CA INDEX NAMES:

CN Hydroperoxide, .alpha.,.alpha.-dimethylbenzyl (8CI)

OTHER NAMES:

CN .alpha.,.alpha.-Dimethylbenzyl hydroperoxide

CN .alpha.-Cumene hydroperoxide

CN .alpha.-Cumyl hydroperoxide

CN 1-Methyl-1-phenylethyl hydroperoxide

CN 2-Hydroperoxy-2-phenylpropane

CN 2-Phenyl-2-propyl hydroperoxide

CN 7-Cumyl hydroperoxide

CN CHP 158

CN Cumen hydroperoxide

CN **Cumene hydroperoxide**

CN Cumenyl hydroperoxide

CN Cumyl hydroperoxide

CN Hyperiz

CN Isopropylbenzene hydroperoxide

CN Kayacumene H

CN Percumyl H

CN Percumyl H 80

CN R 239A

CN Trigonox K 80

CN Trigonox R 239A

CN Trigonox R 239R

FS 3D CONCORD

DR 79568-78-8

MF C9 H12 O2

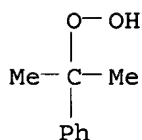
CI COM

LC STN Files: AGRICOLA, ANABSTR, AQUIRE, BEILSTEIN\*, BIOBUSINESS, BIOSIS, BIOTECHNO, CA, CANCERLIT, CAOLD, CAPLUS, CASREACT, CBNB, CEN, CHEMCATS, CHEMINFORMRX, CHEMLIST, CIN, CSCHM, CSNB, DDFU, DETHERM\*, DIPPR\*, DRUGU, EMBASE, ENCOMPLIT, ENCOMPLIT2, ENCOMPPAT, ENCOMPPAT2, GMELIN\*, HODOC\*, HSDB\*, IFICDB, IFIPAT, IFIUDB, MEDLINE, MSDS-OHS, NIOSHTIC, PDLCOM\*, PIRA, PROMT, RTECS\*, SPECINFO, SYNTHLINE, TOXCENTER, USPAT2, USPATFULL, VTB

(\*File contains numerically searchable property data)

Other Sources: DSL\*\*, EINECS\*\*, TSCA\*\*

(\*\*Enter CHEMLIST File for up-to-date regulatory information)



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

4686 REFERENCES IN FILE CA (1967 TO DATE)

39 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA

4690 REFERENCES IN FILE CAPLUS (1967 TO DATE)

28 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

=> s cumene hydroperoxide

657 CUMENE

5406 HYDROPEROXIDE

4 HYDROPEROXIDES

5406 HYDROPEROXIDE

(HYDROPEROXIDE OR HYDROPEROXIDES)

L2 25 CUMENE HYDROPEROXIDE

(CUMENE(W)HYDROPEROXIDE)

```
=> s l2 and water
      2160 WATER
      78 WATERS
      2238 WATER
      (WATER OR WATERS)
L3      0 L2 AND WATER
```

```
=> s l2 and h20
      244 H20
L4      0 L2 AND H20
```

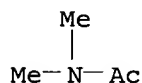
```
=> d scan ;2
L4 HAS NO ANSWERS
```

2 IS NOT A RECOGNIZED COMMAND  
 The previous command name entered was not recognized by the system.  
 For a list of commands available to you in the current file, enter  
 "HELP COMMANDS" at an arrow prompt (=>).

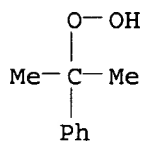
```
=> d scan l2
```

```
L2  25 ANSWERS  REGISTRY  COPYRIGHT 2002 ACS
IN  Acetamide, N,N-dimethyl-, compd. with 1-methyl-1-phenylethyl hydroperoxide
    (1:1) (9CI)
MF  C9 H12 O2 . C4 H9 N O

    CM  1
```

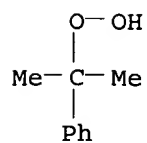


```
CM  2
```



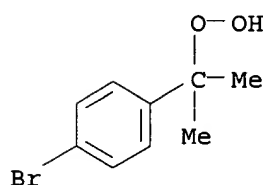
HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):10

```
L2  25 ANSWERS  REGISTRY  COPYRIGHT 2002 ACS
IN  Hydroperoxide, 1-methyl-1-phenylethyl, sodium salt (9CI)
MF  C9 H12 O2 . Na
```



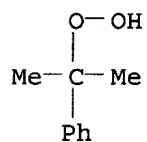
● Na

L2 25 ANSWERS REGISTRY COPYRIGHT 2002 ACS  
 IN Hydroperoxide, 1-(4-bromophenyl)-1-methylethyl (9CI)  
 MF C9 H11 Br O2  
 CI COM



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

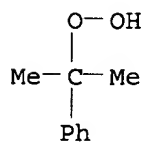
L2 25 ANSWERS REGISTRY COPYRIGHT 2002 ACS  
 IN Hydroperoxide, 1-methyl-1-phenylethyl (9CI)  
 MF C9 H12 O2  
 CI COM



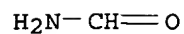
\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L2 25 ANSWERS REGISTRY COPYRIGHT 2002 ACS  
 IN Formamide, compd. with 1-methyl-1-phenylethyl hydroperoxide (1:1) (9CI)  
 MF C9 H12 O2 . C H3 N O

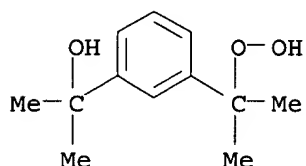
CM 1



CM 2

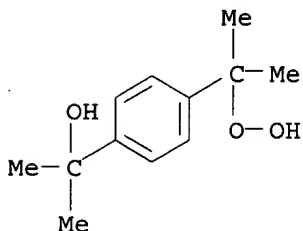


L2 25 ANSWERS REGISTRY COPYRIGHT 2002 ACS  
 IN Benzenemethanol, 3-(1-hydroperoxy-1-methylethyl)-.alpha.,.alpha.-dimethyl-  
 (9CI)  
 MF C12 H18 O3



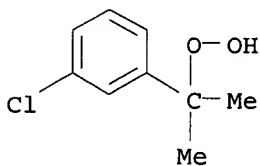
\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L2 25 ANSWERS REGISTRY COPYRIGHT 2002 ACS  
 IN Benzenemethanol, 4-(1-hydroperoxy-1-methylethyl)-.alpha.,.alpha.-dimethyl-  
 (9CI)  
 MF C12 H18 O3



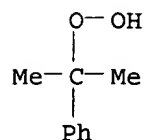
\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L2 25 ANSWERS REGISTRY COPYRIGHT 2002 ACS  
 IN Hydroperoxide, 1-(3-chlorophenyl)-1-methylethyl (9CI)  
 MF C9 H11 Cl O2  
 CI COM



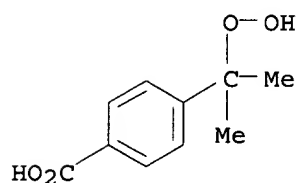
\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L2 25 ANSWERS REGISTRY COPYRIGHT 2002 ACS  
 IN Hydroperoxide, 1-methyl-1-phenylethyl, potassium salt (9CI)  
 MF C9 H12 O2 . K



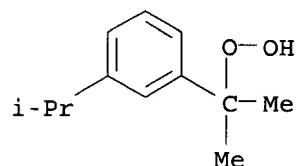
● K

L2 25 ANSWERS REGISTRY COPYRIGHT 2002 ACS  
 IN Benzoic acid, 4-(1-hydroperoxy-1-methylethyl)- (9CI)  
 MF C10 H12 O4  
 CI COM



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L2 25 ANSWERS REGISTRY COPYRIGHT 2002 ACS  
 IN Hydroperoxide, 1-methyl-1-[3-(1-methylethyl)phenyl]ethyl (9CI)  
 MF C12 H18 O2



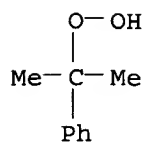
\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):10

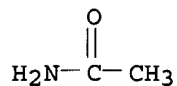
L2 25 ANSWERS REGISTRY COPYRIGHT 2002 ACS  
 IN Acetamide, compd. with 1-methyl-1-phenylethyl hydroperoxide (1:1) (9CI)  
 MF C9 H12 O2 . C2 H5 N O

CM 1

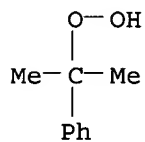




CM 2

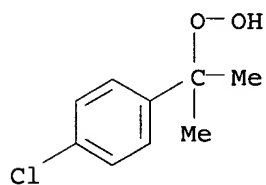


L2 25 ANSWERS REGISTRY COPYRIGHT 2002 ACS  
 IN Hydroperoxide, 1-methyl-1-phenylethyl, lithium salt (9CI)  
 MF C9 H12 O2 . Li



● Li

L2 25 ANSWERS REGISTRY COPYRIGHT 2002 ACS  
 IN Hydroperoxide, 1-(4-chlorophenyl)-1-methylethyl (9CI)  
 MF C9 H11 Cl O2  
 CI COM

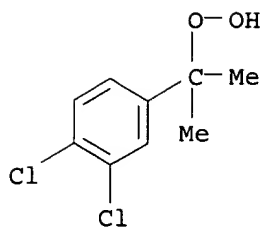


\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L2 25 ANSWERS REGISTRY COPYRIGHT 2002 ACS  
 IN **Pitch, phenol manuf. cumene hydroperoxide oxidn.**  
 MF Unspecified  
 CI MAN, CTS

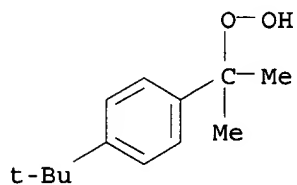
\*\*\* STRUCTURE DIAGRAM IS NOT AVAILABLE \*\*\*

L2 25 ANSWERS REGISTRY COPYRIGHT 2002 ACS  
 IN Hydroperoxide, 1-(3,4-dichlorophenyl)-1-methylethyl (9CI)  
 MF C9 H10 Cl2 O2



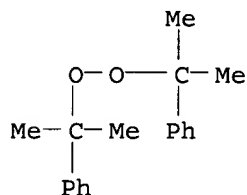
\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L2 25 ANSWERS REGISTRY COPYRIGHT 2002 ACS  
 IN Hydroperoxide, 1-[4-(1,1-dimethylethyl)phenyl]-1-methylethyl (9CI)  
 MF C13 H20 O2  
 CI COM



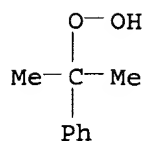
\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L2 25 ANSWERS REGISTRY COPYRIGHT 2002 ACS  
 IN Peroxide, bis(1-methyl-1-phenylethyl) (9CI)  
 ADDITIONAL NAMES NOT AVAILABLE IN THIS FORMAT  
 MF C18 H22 O2  
 CI COM

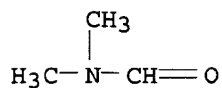


\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

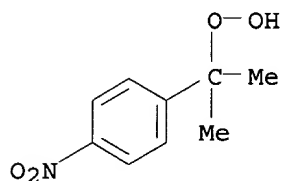
L2 25 ANSWERS REGISTRY COPYRIGHT 2002 ACS  
 IN Formamide, N,N-dimethyl-, compd. with 1-methyl-1-phenylethyl hydroperoxide  
 (1:1) (9CI)  
 MF C9 H12 O2 . C3 H7 N O  
 CM 1



CM 2

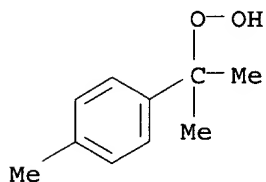


L2 25 ANSWERS REGISTRY COPYRIGHT 2002 ACS  
 IN Hydroperoxide, 1-methyl-1-(4-nitrophenyl)ethyl (9CI)  
 MF C9 H11 N O4  
 CI COM



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

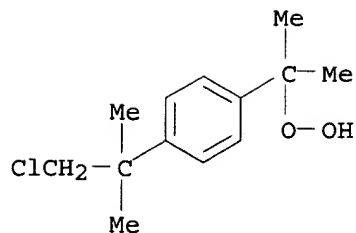
L2 25 ANSWERS REGISTRY COPYRIGHT 2002 ACS  
 IN Hydroperoxide, 1-methyl-1-(4-methylphenyl)ethyl (9CI)  
 MF C10 H14 O2  
 CI COM



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

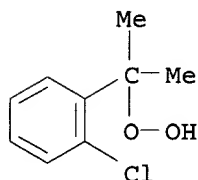
HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):10

L2 25 ANSWERS REGISTRY COPYRIGHT 2002 ACS  
 IN Hydroperoxide, 1-[4-(2-chloro-1,1-dimethylethyl)phenyl]-1-methylethyl  
 (9CI)  
 MF C13 H19 Cl O2  
 CI COM



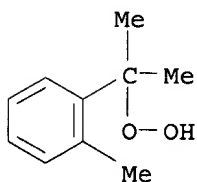
\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L2 25 ANSWERS REGISTRY COPYRIGHT 2002 ACS  
 IN Hydroperoxide, 1-(2-chlorophenyl)-1-methylethyl (9CI)  
 MF C9 H11 Cl O2



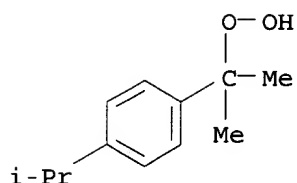
\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L2 25 ANSWERS REGISTRY COPYRIGHT 2002 ACS  
 IN Hydroperoxide, 1-methyl-1-(2-methylphenyl)ethyl (9CI)  
 MF C10 H14 O2



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L2 25 ANSWERS REGISTRY COPYRIGHT 2002 ACS  
 IN Hydroperoxide, 1-methyl-1-[4-(1-methylethyl)phenyl]ethyl (9CI)  
 MF C12 H18 O2



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

ALL ANSWERS HAVE BEEN SCANNED

=> file caplus

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

22.34

22.95

FILE 'CAPLUS' ENTERED AT 17:22:28 ON 05 SEP 2002

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FILE COVERS 1907 - 5 Sep 2002 VOL 137 ISS 10

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=> d his

(FILE 'HOME' ENTERED AT 17:20:54 ON 05 SEP 2002)

FILE 'CAPLUS' ENTERED AT 17:21:16 ON 05 SEP 2002

FILE 'REGISTRY' ENTERED AT 17:21:28 ON 05 SEP 2002

```
L1      1 S CUMENE HYDROPEROXIDE/CN
L2      25 S CUMENE HYDROPEROXIDE
L3      0 S L2 AND WATER
L4      0 S L2 AND H2O
```

FILE 'CAPLUS' ENTERED AT 17:22:28 ON 05 SEP 2002

=> s l1 and weight percent water  
4694 L1

```

      87965 WEIGHT
      7555 WEIGHTS
      93397 WEIGHT
            (WEIGHT OR WEIGHTS)
      1272657 WT
      94563 WTS
      1321531 WT
            (WT OR WTS)
      1348119 WEIGHT
            (WEIGHT OR WT)
      67923 PERCENT
      1267 PERCENTS
      68985 PERCENT
            (PERCENT OR PERCENTS)
      1940411 WATER
      212506 WATERS
      1991062 WATER
            (WATER OR WATERS)
      32 WEIGHT PERCENT WATER
            (WEIGHT(W) PERCENT(W) WATER)
L5      0 L1 AND WEIGHT PERCENT WATER

=> s l1 (1) (water or h2o)
      4694 L1
      1940411 WATER
      212506 WATERS
      1991062 WATER
            (WATER OR WATERS)
      918284 H2O
L6      118 L1 (L) (WATER OR H2O)

=> s cumene?/ti
L7      2029 CUMENE?/TI

=> s l6 and l7
L8      10 L6 AND L7

=> d ti 1-10

L8      ANSWER 1 OF 10  CAPLUS  COPYRIGHT 2002 ACS
TI      Process for separating phenol from a mixture comprising at least
hydroxyacetone, cumene, water and phenol

L8      ANSWER 2 OF 10  CAPLUS  COPYRIGHT 2002 ACS
TI      Preparation of environmentally safe, water-diluted cumene
hydroperoxide solutions

L8      ANSWER 3 OF 10  CAPLUS  COPYRIGHT 2002 ACS
TI      Procedure for the recovery of cumene hydroperoxide from
hydroperoxide-containing, phenol-manufacture process waste water by
extraction with cumene

L8      ANSWER 4 OF 10  CAPLUS  COPYRIGHT 2002 ACS
TI      Water-alkaline emulsion cumene oxidation process

L8      ANSWER 5 OF 10  CAPLUS  COPYRIGHT 2002 ACS
TI      Reliability and hazards analysis of a cumene hydroperoxide plant

L8      ANSWER 6 OF 10  CAPLUS  COPYRIGHT 2002 ACS
TI      Oxidation of cumene in the presence of water additives

L8      ANSWER 7 OF 10  CAPLUS  COPYRIGHT 2002 ACS
TI      Chromatographic determination of water and phenol in products from the
manufacture of phenol and acetone by the cumene hydroperoxide

```

process

L8 ANSWER 8 OF 10 CAPLUS COPYRIGHT 2002 ACS

TI Cumene hydroperoxide

L8 ANSWER 9 OF 10 CAPLUS COPYRIGHT 2002 ACS

TI Study of intermolecular interactions in the cumene hydroperoxide-water system by the proton magnetic resonance method

L8 ANSWER 10 OF 10 CAPLUS COPYRIGHT 2002 ACS

TI Study of the decomposition of cumene hydroperoxide in the presence of different inhibitors during production of butadiene-styrene rubbers

=> d ibib abs hitstr 1-10

L8 ANSWER 1 OF 10 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 2002:429321 CAPLUS

DOCUMENT NUMBER: 136:403494

TITLE: Process for separating phenol from a mixture comprising at least hydroxyacetone, cumene, water and phenol

INVENTOR(S): Schwarz, Christoph; Weber, Mark; Tanger, Uwe; Korte, Hermann-Josef; Ullrich, Jochen

PATENT ASSIGNEE(S): Phenolchemie G.m.b.H. & Co. K.-G., Germany

SOURCE: U.S. Pat. Appl. Publ., 9 pp.

CODEN: USXXCO

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2002066661	A1	20020606	US 2001-970856	20011005
WO 2002046133	A1	20020613	WO 2001-EP14029	20011130
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM			
RW:	GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			

PRIORITY APPLN. INFO.: DE 2000-10060505 A 20001206

AB Phenol is sepd. from a mixt. contg. hydroxyacetone, cumene, H2O and phenol, by fractionating the mixt. in a process with a fractional distn. step and a phase sepn. step to provide a single phenol fraction contg. <300 ppm of hydroxyacetone. In the work-up by distn. of cleavage product mixts., the hydroxyacetone can be removed from the cleavage product mixt. together with a phenol fraction from which the hydroxyacetone has to be removed. A process can be used for purifying cleavage product mixts. obtained in the cleavage of alkylaryl hydroperoxides such as cumene hydroperoxide. The process allows sepn. of phenol and acetone from mixts. obtained in the cleavage of cumene hydroperoxide.

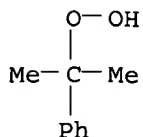
IT 80-15-9, Cumene hydroperoxide

RL: CAT (Catalyst use); USES (Uses)

(process for sepg. phenol from a mixt. comprising at least hydroxyacetone, cumene, water and phenol)

RN 80-15-9 CAPLUS

CN Hydroperoxide, 1-methyl-1-phenylethyl (9CI) (CA INDEX NAME)



L8 ANSWER 2 OF 10 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 2002:220548 CAPLUS

DOCUMENT NUMBER: 136:264830

TITLE: Preparation of environmentally safe, water-diluted cumene hydroperoxide solutions

INVENTOR(S): Henry, Keith E.; Aiken, John E.

PATENT ASSIGNEE(S): Aristech Chemical Corporation, USA

SOURCE: PCT Int. Appl., 16 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002022570	A2	20020321	WO 2001-US28123	20010904
WO 2002022570	A3	20020704		
W: AU, CA, JP, KR, MX, NO, RU				
RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR				
AU 2001088913	A5	20020326	AU 2001-88913	20010904
PRIORITY APPLN. INFO.:			US 2000-660099	A 20000912
			WO 2001-US28123	W 20010904

AB The use of water, rather than cumene, as a more environmentally acceptable diluent for purified cumene hydroperoxide (CHP) solns. is described. From 1-6% water can be used to dil. purified CHP solns., thus reducing or eliminating the use of the hazardous compd. cumene as a diluent. This method and the CHP-water solns. significantly reduce or eliminate the hazardous emissions problems encountered with the use of cumene as a diluent and make CHP solns. more environmentally acceptable to produce, transport, and use. Water as a diluent also depresses the f.p. of the resultant soln., thus enabling year-round use of higher-concn. CHP solns. Water-dild. CHP solns. also reduce cumene-related impurities in finished products made from them.

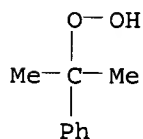
IT 80-15-9, Cumene hydroperoxide

RL: PEP (Physical, engineering or chemical process); PRP (Properties); PYP (Physical process); TEM (Technical or engineered material use); PROC (Process); USES (Uses)

(prepn. of safe water-dild. cumene hydroperoxide solns.)

RN 80-15-9 CAPLUS

CN Hydroperoxide, 1-methyl-1-phenylethyl (9CI) (CA INDEX NAME)



L8 ANSWER 3 OF 10 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 2000:188382 CAPLUS

DOCUMENT NUMBER: 132:209457



TITLE: Procedure for the recovery of **cumene** hydroperoxide from hydroperoxide-containing, phenol-manufacture process waste water by extraction with **cumene**

INVENTOR(S): Hofmann, Guenter; Pester, Rolf; Bartkowiak, Horst

PATENT ASSIGNEE(S): Domo Caproleuna G.m.b.H., Germany

SOURCE: Ger., 6 pp.  
CODEN: GWXXAW

DOCUMENT TYPE: Patent

LANGUAGE: German

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 19846508	C1	20000323	DE 1998-19846508	19981009
EP 997456	A1	20000503	EP 1999-119594	19991002

R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO

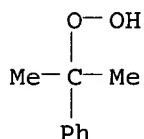
PRIORITY APPLN. INFO.: DE 1998-19846508 19981009

AB Cumene hydroperoxide is recovered from hydroperoxide-contg., phenol-manuf. process waste water by extn. of the water with cumene (cumol) which is formed during phenol manuf. The waste water resulting after the extn. contains only traces of cumene hydroperoxide and exhibits almost no removal of the residual Me hydroperoxide.

IT **80-15-9P**, Cumene hydroperoxide  
RL: PEP (Physical, engineering or chemical process); PUR (Purification or recovery); PREP (Preparation); PROC (Process)  
(procedure for the recovery of cumene hydroperoxide from hydroperoxide-contg. phenol-manuf. process waste **water** by extn. with cumol)

RN 80-15-9 CAPLUS

CN Hydroperoxide, 1-methyl-1-phenylethyl (9CI) (CA INDEX NAME)



REFERENCE COUNT: 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 4 OF 10 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1998:116085 CAPLUS

DOCUMENT NUMBER: 128:129491

TITLE: Water-alkaline emulsion **cumene** oxidation process

INVENTOR(S): Zakoshansky, Vladimir Michailo; Griaznov, Andrei K.; Vasilieva, Irina Ivanovna; Fulmer, John William; Kight, William Dale

PATENT ASSIGNEE(S): General Electric Co., USA

SOURCE: Eur. Pat. Appl., 13 pp.

CODEN: EPXXDW

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 816335	A1	19980107	EP 1997-304341	19970620

EP 816335 B1 20011031  
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,  
IE, FI

US 5767322	A	19980616	US 1996-670304	19960627
ES 2163102	T3	20020116	ES 1997-304341	19970620
CN 1173491	A	19980218	CN 1997-114047	19970624
CN 1088059	B	20020724		
JP 10087609	A2	19980407	JP 1997-167816	19970625
US 5908962	A	19990601	US 1998-20395	19980209

PRIORITY APPLN. INFO.: US 1996-670304 A 19960627

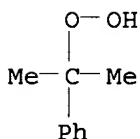
AB Greater efficiency in the title process using a cascade of reactors is obtained by splitting the reactor cascade into 2 stages with the 1st stage utilizing  $\text{NH}_4\text{NaCO}_3$  as the active carbonate in the stage contg. .ltoreq.18% cumene hydroperoxide (I) and using  $\text{Na}_2\text{CO}_3$  as the active carbonate in the stage contg. .gtoreq.18% I. By directly injecting ammonia into a recycle stream org. acids are efficiently neutralized. A counter current water wash of the 2nd stage also increases process efficiency by scrubbing out unwanted impurities. Control of pH in the process improves efficiency and reduces impurity levels.

IT 80-15-9P, Cumene hydroperoxide

RL: IMF (Industrial manufacture); PREP (Preparation)  
(~~water~~-alk. emulsion cumene oxidn. process with good efficiency)

RN 80-15-9 CAPLUS

CN Hydroperoxide, 1-methyl-1-phenylethyl (9CI) (CA INDEX NAME)



L8 ANSWER 5 OF 10 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1986:429162 CAPLUS

DOCUMENT NUMBER: 105:29162

TITLE: Reliability and hazards analysis of a **cumene** hydroperoxide plant

AUTHOR(S): Arendt, J. S.; Casada, M. L.; Rooney, J. J.

CORPORATE SOURCE: JBF Assoc. Inc., Knoxville, TN, 37932, USA

SOURCE: Plant/Oper. Prog. (1986), 5(2), 97-102

CODEN: POPPDE; ISSN: 0278-4513

DOCUMENT TYPE: Journal

LANGUAGE: English

AB An anal. of reliability and risk of a cumene hydroperoxide [ 80-15-9] plant led to conclusions that call for the updating of the existing emergency procedures dealing with the oxidizers, inspections and testing of important safety equipment on a regular basis, shortening the closure time delay of the main process air valve in case of a power outage, and a modification of the existing emergency procedures for the diesel cooling **water** system.

L8 ANSWER 6 OF 10 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1984:67930 CAPLUS

DOCUMENT NUMBER: 100:67930

TITLE: Oxidation of **cumene** in the presence of water additives

AUTHOR(S): Golyshcheva, G. P.; Ionova, M. V.; Il'ina, T. A.; Vasil'ev, V. F.

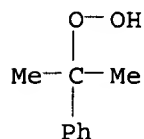
CORPORATE SOURCE: Vses. Nauchno-Issled. Inst. Org. Sint.,

Novokuibyshevsk, USSR

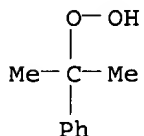
SOURCE: Neftepererab. Neftekhim. (Moscow) (1983), (12), 31

CODEN: NNNSAF; ISSN: 0028-1190

DOCUMENT TYPE: Journal  
LANGUAGE: Russian  
AB Addn. of H<sub>2</sub>O to a cumene oxidn. system increased the rate of cumene hydroperoxide formation but lowered the selectivity.  
IT **80-15-9P**  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(prepn. of, effect of **water** on)  
RN 80-15-9 CAPLUS  
CN Hydroperoxide, 1-methyl-1-phenylethyl (9CI) (CA INDEX NAME)



L8 ANSWER 7 OF 10 CAPLUS COPYRIGHT 2002 ACS  
ACCESSION NUMBER: 1983:624444 CAPLUS  
DOCUMENT NUMBER: 99:224444  
TITLE: Chromatographic determination of water and phenol in products from the manufacture of phenol and acetone by the **cumene** hydroperoxide process  
AUTHOR(S): Bruk, A. Yu.; Gaishun, K. A.; Markova, V. A.  
CORPORATE SOURCE: Grozn. KhZ, Grozny, USSR  
SOURCE: Neftepererab. Neftekhim. (Moscow) (1983), (10), 23-4  
CODEN: NNNSAF; ISSN: 0028-1190  
DOCUMENT TYPE: Journal  
LANGUAGE: Russian  
AB H<sub>2</sub>O and PhOH were detd. by gas chromatog. with thermal-cond. and flame-ionization detectors, resp. Various products were analyzed, such as Me<sub>2</sub>CO, phenol-formaldehyde resin, Syntan 2 tanning agent, and the reaction mass from the decompn. of cumene hydroperoxide. The sepn. was carried out at 130.degree. on a 50 .times. 0.3-cm column packed with Polysorb 1 coated with 5 wt.% Tween 80.  
IT **80-15-9D**, decompn. products  
RL: ANST (Analytical study)  
(phenol and **water** detn. in, gas chromatog.)  
RN 80-15-9 CAPLUS  
CN Hydroperoxide, 1-methyl-1-phenylethyl (9CI) (CA INDEX NAME)



L8 ANSWER 8 OF 10 CAPLUS COPYRIGHT 2002 ACS  
ACCESSION NUMBER: 1982:144912 CAPLUS  
DOCUMENT NUMBER: 96:144912  
TITLE: **Cumene** hydroperoxide  
INVENTOR(S): Franke, Christiane; Fuhrmann, Guenther; Haase, Bernd; Hager, Werner; Hofmann, Rolf; Naumann, Hans Joachim; Raue, Bernd  
PATENT ASSIGNEE(S): VEB Leuna-Werke "Walter Ulbricht", Ger. Dem. Rep.  
SOURCE: Ger. (East), 10 pp.  
CODEN: GEXXA8  
DOCUMENT TYPE: Patent

LANGUAGE: German  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
	DD 151000	T	19810930	DD 1979-212412	19790423
AB	cumene [98-82-8] Is oxidized to prep. cumene hydroperoxide (I) [80-15-9], and the unreacted cumene is sepd. by distn., washed with <b>water</b> to remove org. acids (esp. HCO <sub>2</sub> H), and recycled to the oxidn. step. Addnl. I is extd. from the <b>water</b> with cumene. The method increases the yield of I, decreases the formation of by-products, and minimizes the deposition of insol. materials on surfaces in the app. The I is used to prep. phenol and acetone. Thus, 54,100 parts oxidn. products contg. I 20.6, PhCMe <sub>2</sub> OH 1.4, and PhAc 0.19% was distd. to sep. 11,000 parts I contg. <100 ppm org. acids, and the cumene (contg. 110 parts org. acid, calcd. as HCO <sub>2</sub> H) was washed with 1600 parts <b>water</b> , mixed with 870 parts cumene and 1.9 parts 15% aq. NaOH, and recycled to the oxidn. step. The <b>water</b> was extd. with 200 parts cumene to recover 8 parts I, giving waste <b>water</b> contg. <2000 ppm I. The oxidn. and distn. app. required cleaning after 1 yr, compared with 350 h when the recycled cumene was not washed with <b>water</b> .				

L8 ANSWER 9 OF 10 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1977:600365 CAPLUS

DOCUMENT NUMBER: 87:200365

TITLE: Study of intermolecular interactions in the **cumene** hydroperoxide-water system by the proton magnetic resonance method

AUTHOR(S): Markaryan, Sh. A.; Beileryan, N. M.; Grigoryan, S. K.

CORPORATE SOURCE: Erevan. Gos. Univ., Yerevan, USSR

SOURCE: Zh. Fiz. Khim. (1977), 51(9), 2385-7  
CODEN: ZFKHA9

DOCUMENT TYPE: Journal

LANGUAGE: Russian

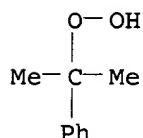
AB NMR data indicated that in the title system proton exchange occurs between PhCMe<sub>2</sub>OOH (I) and H<sub>2</sub>O. At 97:3 I-H<sub>2</sub>O the rate const. for this exchange is 85 s<sup>-1</sup>. Interactions between the .pi. system of I and H<sub>2</sub>O also occur.

IT 80-15-9

RL: PRP (Properties)  
(interaction of, with **water**)

RN 80-15-9 CAPLUS

CN Hydroperoxide, 1-methyl-1-phenylethyl (9CI) (CA INDEX NAME)



L8 ANSWER 10 OF 10 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1977:30764 CAPLUS

DOCUMENT NUMBER: 86:30764

TITLE: Study of the decomposition of **cumene** hydroperoxide in the presence of different inhibitors during production of butadiene-styrene rubbers

AUTHOR(S): Titov, A. P.; Papkov, V. N.; Smol'yaninova, T. S.

CORPORATE SOURCE: USSR

SOURCE: Zh. Prikl. Khim. (Leningrad) (1976), 49(9), 2041-3  
CODEN: ZPKHAB

DOCUMENT TYPE: Journal

LANGUAGE: Russian

AB The inhibition of emulsion polymn. initiated by cumene hydroperoxide (I) [80-15-9]-redox system by inhibitors [Na N,N-dimethyldithiocarbamate (II) [128-04-1], NaNO<sub>2</sub>, p-hydroxydiphenylamine (III) [122-37-2], hydroxylamine (IV) [7803-49-8] N,N-diethylhydroxylamine (V) [3710-84-7], or dibenzylhydroxylamine (VI) [621-07-8]] is due in part to the decompn. of I by these inhibitors and in part to the chain termination reactions in which these inhibitors participate. The foregoing was demonstrated by detg. the kinetics of I decompn. in media modelling the emulsions used in prepn. of SBR. These media contained I, redox system, PhMe (substituted for monomers), and water. The effectiveness of I decompn. decreased in the series: V > III > IV > VI > NaNO<sub>2</sub> > II which did not correspond exactly to the effectiveness of arresting the formation of SBR in emulsion copolymns.

=> file merck

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

52.96

75.91

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE

TOTAL

ENTRY

SESSION

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-6.20

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L9 0 L1

=> d his

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FILE 'CAPLUS' ENTERED AT 17:21:16 ON 05 SEP 2002

FILE 'REGISTRY' ENTERED AT 17:21:28 ON 05 SEP 2002

L1 1 S CUMENE HYDROPEROXIDE/CN

L2 25 S CUMENE HYDROPEROXIDE

L3 0 S L2 AND WATER

L4 0 S L2 AND H2O

FILE 'CAPLUS' ENTERED AT 17:22:28 ON 05 SEP 2002

L5 0 S L1 AND WEIGHT PERCENT WATER

L6 118 S L1 (L) (WATER OR H2O)

L7 2029 S CUMENE?/TI

L8 10 S L6 AND L7

FILE 'MRCK' ENTERED AT 17:26:43 ON 05 SEP 2002

L9 0 S L1

=> file beilstein  
COST IN U.S. DOLLARS

SINCE FILE	TOTAL
ENTRY	SESSION
0.30	76.21

FULL ESTIMATED COST

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE	TOTAL
ENTRY	SESSION
0.00	-6.20

CA SUBSCRIBER PRICE

FILE 'BEILSTEIN' ENTERED AT 17:27:00 ON 05 SEP 2002

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<http://info.cas.org/ONLINE/DBSS/beilsteinss.html> <<<

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documents use "/XXX.RX".)  
For additional information see HELP RXS. <<<

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L10 1 L1

=> d aze

L10 ANSWER 1 OF 1 BEILSTEIN COPYRIGHT 2002 BEILSTEIN CDS MDL

Azeotrope (MCS):  
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QRD ----- Query Related Data (IDE plus HIT)  
IDE ----- Identification of Substance, plus Structure  
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ALL ----- All Display fields (Lengthy display!)  
CHE ----- Chemical Data  
PHY ----- Physical Data

HIT ----- All fields containing hit terms  
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prompt, e.g. => HELP FORMAT.  
ENTER DISPLAY FORMAT (QRD):end

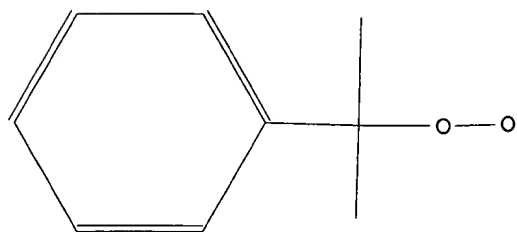
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L10 ANSWER 1 OF 1 BEILSTEIN COPYRIGHT 2002 BEILSTEIN CDS MDL

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Beilstein Records (BRN):      1908117
Beilstein Pref. RN (BPR):    80-15-9
CAS Reg. No. (RN):          80-15-9
Chemical Name (CN):          1-methyl-1-phenyl-ethyl hydroperoxide,
                             1-Methyl-1-phenyl-aethylhydroperoxid,
                             .alpha.,.alpha.-dimethylbenzyl
                             hydroperoxide, cumene hydroperoxide,
                             .alpha.-cumyl hydroperoxide
Autonom Name (AUN):          1-methyl-1-phenyl-ethyl hydroperoxide
Molec. Formula (MF):          C9 H12 O2
Molecular Weight (MW):        152.19
Lawson Number (LN):           5240
Compound Type (CTYPE):        isocyclic
Constitution ID (CONSID):      1754219
Tautomer ID (TAUTID):          1833317
Beilstein Citation (BSO):      3-06-00-01814, 4-06-00-03221, 5-06, 6-06
Entry Date (DED):             1989/06/29
Update Date (DUPD):           2001/07/25

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# Field Availability:

Code	Name	Occurrence
BRN	Beilstein Records	1
BPR	Beilstein Preferred RN	1
RN	CAS Registry Number	1
CN	Chemical Name	5
AUN	Autonomname	1
MF	Molecular Formula	1
FW	Formular Weight	1
LN	Lawson Number	1
CTYPE	Compound Type	1
CONSID	Constitution ID	1
TAUTID	Tautomer ID	1
BSO	Beilstein Citation	4

ED	Entry Date	1
UPD	Update Date	1
ASSM	Association (MCS)	25
BP	Boiling Point	33
CDER	Chemical Derivative	31
DE	Dissociation Exponent	4
DEN	Density (Liquid)	6
DM	Dipole Moment	3
DP	Decomposition Point	1
ECTOX	Ecotoxicology	8
ELCB	Electrochemical Behaviour	1
ESR	ESR Data	2
FINFO	Further Information	2
HVAP	Enthalpy of Vaporization	1
IR	Infrared Spectrum	9
LLSM	Liquid/Liquid System (MCS)	8
LUM	Luminescence	1
MP	Melting Point	2
MS	Mass Spectrum	1
NMR	Nuclear Magnetic Resonance	20
OTHE	Other Thermochemical Data	1
PHARM	Pharmacological Data	92
RAS	Raman Spectrum	3
RI	Refractive Index	20
RSTR	Related Structure	1
SLB	Solubility (MCS)	3
SOLM	Solution Behaviour (MCS)	1
TRAM	Transport Phenomena (MCS)	1
USC	Use of Compound	1
UVS	UV and Visible Spectrum	3
XREF	Crossfile Reference	10

This substance also occurs in Reaction Documents:

Code	Name	Occurrence
=====		
RX	Reaction Documents	301
RXREA	Substance is Reaction Reactant	276
RXPRO	Substance is Reaction Product	25

=> d frxpro

L10 ANSWER 1 OF 1 BEILSTEIN COPYRIGHT 2002 BEILSTEIN CDS MDL

Reaction:

RX

Reaction ID: 8753725  
 Reactant BRN: 2454403  
 Reactant: Perbuttersaeure-cumolester  
 Product BRN: 1908117  
 Product: 1-methyl-1-phenyl-ethyl hydroperoxide  
 No. of Reaction Details: 1

Reaction Details:

RX

Reaction RID: 8753725.1  
 Reaction Classification: Preparation  
 Reagent: (n-Bu3Sn)2O  
 Solvent: diethyl ether  
 Time: 30 hour(s)  
 Temperature: 25 Cel  
 Reference(s):



1. Baj, Stefan; Chrobok, Anna, Syn.Lett.  
, CODEN: SYNLES(5), <2001>, 623 - 624; BABS-6282951

Reaction:

RX

Reaction ID: 8612643  
Reactant BRN: 1236613  
Reactant: isopropylbenzene  
Product BRN: 1905012, 1908117, 1905601, 969405  
Product: 2-phenyl-propan-2-ol, 1-methyl-1-phenyl-ethyl hydroperoxide, 2-phenyl-propionaldehyde, isopropenylbenzene  
Stoichiometric Equation: 1236613 \*4  
No. of Reaction Details: 1

Reaction Details:

RX

Reaction RID: 8612643.1  
Reaction Classification: Chemical behaviour  
Reagent: Fe(TPFPP)Cl, O2  
Solvent: various solvent(s)  
Temperature: 100 Cel  
Subject Studied: Product distribution  
Reaction Type: Oxidation  
Prototype Reaction: Further Variations:, reaction times  
Reference(s):  
1. Evans, Steven; Smith, John R. Lindsay, J.Chem.Soc.Perkin Trans.2,  
CODEN: JCPKBH(7), <2000>, 1541 - 1552; BABS-6248901

Reaction:

RX

Reaction ID: 7160212  
Reactant: cumene (1-methyl-1-phenyl-ethyl hydroperoxide containing)  
Product BRN: 1908117  
Product: 1-methyl-1-phenyl-ethyl hydroperoxide  
No. of Reaction Details: 10

Reaction Details:

RX

Reaction RID: 7160212.1  
Reaction Classification: Preparation (half reaction)  
Reagent: benzoic acid, oxygen  
Note(s): Handbook  
Reference(s):  
1. Patent: Soc. Usines Chim. Rhone-Poulenc US 2697121 1952

RX

Reaction RID: 7160212.2  
Reaction Classification: Preparation (half reaction)  
Reagent: copper phthalocyanin, oxygen  
Note(s): Handbook  
Reference(s):

1. Hock; Kropf, J.Prakt.Chem., CODEN: JPCEAO, <4> 9, <1959>, 173, 176, 184

RX

Reaction RID: 7160212.3  
Reaction Classification: Preparation (half reaction)  
Reagent: NH3, oxygen  
Note(s): Handbook  
Reference(s):  
1. Patent: Hercules Powder Co. US 2632026 1950

RX

Reaction RID: 7160212.4  
Reaction Classification: Preparation (half reaction)  
Reagent: aqueous NaOH, oxygen

Note(s): Handbook  
Reference(s):  
1. Patent: Hercules Powder Co. US 2663740 1952  
2. Patent: Distillers Co. DE 924449 1948, DRP/DRBP Org.Chem.

RX

Reaction RID: 7160212.5  
Reaction Classification: Preparation (half reaction)  
Reagent: Na<sub>2</sub>CO<sub>3</sub>, oxygen  
Note(s): Handbook  
Reference(s):  
1. Patent: ICI US 2796439 1954

RX

Reaction RID: 7160212.6  
Reaction Classification: Preparation (half reaction)  
Reagent: aqueous formaldehyde, oxygen  
Note(s): Handbook  
Reference(s):  
1. Patent: Soc. Usines Chim. Rhone-Poulenc US 2680139 1953

RX

Reaction RID: 7160212.7  
Reaction Classification: Preparation (half reaction)  
Reagent: copper formate, oxygen  
Note(s): Handbook  
Reference(s):  
1. Patent: ICI US 2820832 1954

RX

Reaction RID: 7160212.8  
Reaction Classification: Preparation (half reaction)  
Reagent: copper benzoate, oxygen  
Note(s): Handbook  
Reference(s):  
1. Patent: ICI US 2820832 1954

RX

Reaction RID: 7160212.9  
Reaction Classification: Preparation (half reaction)  
Reagent: manganese naphthenate, oxygen  
Note(s): Handbook  
Reference(s):  
1. Patent: Hercules Powder Co. US 2664448 1948

RX

Reaction RID: 7160212.10  
Reaction Classification: Preparation (half reaction)  
Reagent: ethanediylldiimino-tetra-acetic acid, oxygen  
Note(s): Handbook  
Reference(s):  
1. Patent: Edogawa Kagaku Kogyo K.K. US 2861107 1956

Reaction:

RX

Reaction ID: 7160211  
Reactant BRN: 2037554, 3587191, 1905012  
Reactant: sulfuric acid, hydrogen peroxide,  
2-phenyl-propan-2-ol  
Product BRN: 1908117  
Product: 1-methyl-1-phenyl-ethyl hydroperoxide  
No. of Reaction Details: 1

Reaction Details:

RX

Reaction RID: 7160211.1  
Reaction Classification: Chemical behaviour  
Other Conditions: 180-markierter 2-Phenyl-propan-2-ol  
Note(s): Handbook  
Reference(s):

1. Bassey et al., J.Chem.Soc., CODEN: JCSOA9, <1955>, 2471, 2473

Reaction:

RX

Reaction ID: 7160210  
Product BRN: 1908117  
Product: 1-methyl-1-phenyl-ethyl hydroperoxide  
No. of Reaction Details: 1

Reaction Details:

RX

Reaction RID: 7160210.1  
Reaction Classification: Preparation (half reaction)  
Reference(s):  
1. Patent: Phenolchemie GmbH DE 1668575 1968, Chem.Abstr., 74(125153m), <1971>  
2. Richardson; Hodge, J.Org.Chem., CODEN: JOCEAH, 35, <1970>, 4012,4013, 4015  
3. Antonovskii et al., Kinet.Catal.(Engl.Transl.), CODEN: KICAA8, 6, <1965>, 736, 815  
4. Patent: Texaco. Devel. Corp. DE 2035504 1970, Chem.Abstr., 76(72223s), <1972>  
5. Min'kov; Keier, Kinet.Catal.(Engl.Transl.), CODEN: KICAA8, 8, <1967>, 133,134,135  
6. Min'kov et al., Kinet.Catal.(Engl.Transl.), CODEN: KICAA8, 8, <1967>, 333  
7. Kulicki; Stec, Roczn.Chem., CODEN: ROCHAC, 50, <1976>, 1075,1076  
8. Solonko et al., Kinet.Katal., CODEN: KNKTA4, 9, <1968>, 631  
9. Solomko et al., Kinet.Katal., CODEN: KNKTA4, 9, <1968>, 815  
10. Ishii et al., Kogyo Kagaku Zasshi, CODEN: KGKZA7, 64, <1961>, 472, Chem.Abstr., 57(7149)  
11. Tanaka; Imamura, Chem.Lett., CODEN: CMLTAG, <1974>, 1347  
12. Tsykskovskii et al., J.Appl.Chem.USSR (Engl.Transl.), CODEN: JAPUAW, 48, <1975>, 2811,2812-2813, Zh.Prikl.Khim.(Leningrad), CODEN: ZPKHAB, 48, <1975>, 2731  
13. Choe; Tsutsumi, Nippon Kagaku Zasshi, CODEN: NPKZAZ, 81, <1960>, 582,583, Chem.Abstr., 56(397), <1962>  
14. Burghardt et al., Zesz.Nauk.Politech.Slask.Chem., CODEN: ZNSCAM, 60, <1972>, 3,4-7,9,10,12-17  
15. Kulicki, Zesz.Nauk.Politech.Slask.Chem., CODEN: ZNSCAM, 36, <1967>, 1,13,19-24,59,61,62  
16. Norikov; Salukvadze, Dokl.Phys.Chem.(Engl.Transl.), CODEN: DKPCAG, 203, <1972>, 254  
17. Choe; Tsutsumi, Nippon Kagaku Zasshi, CODEN: NPKZAZ, 81, <1960>, 582,583-586, Chem.Abstr.(397), <1962>  
18. Wagner, J.Prakt.Chem., CODEN: JPCEAO, 27, <1965>, 297  
19. Maruyama et al., Nippon Kagaku Zasshi, CODEN: NPKZAZ, 85, <1964>, 145, Chem.Abstr., 61(13222), <1964>  
20. Kasmin, J.Appl.Chem.USSR (Engl.Transl.), CODEN: JAPUAW, 35, <1962>, 398, Zh.Prikl.Khim.(Leningrad), CODEN: ZPKHAB, 35, <1962>, 422, Chem.Abstr., 57(700), <1962>  
21. Patent: Etienne; Le Berre FR 1239348, Chem.Abstr., 56(3415), <1962>  
22. Wagner, Z.Chem., CODEN: ZECEAL, 5, <1965>, 73  
23. Kropf, Justus Liebig's Ann. Chem., CODEN: JLACBF, 637, <1960>, 73,76,92  
24. Kropf; Knabjohann, Justus Liebig's Ann. Chem., CODEN: JLACBF, 739, <1970>, 95,98,99  
25. Kulicki; Stec, Roczn.Chem., CODEN: ROCHAC, 45, <1971>, 601,603  
26. Rouchaud, Bull.Soc.Chim.Belg., CODEN: BSCBAG, 76, <1967>, 171,184  
27. Rouchaud, Bull.Soc.Chim.Belg., CODEN: BSCBAG, 76, <1967>, 186  
28. Gadelle; Clement, Bull.Soc.Chim.Fr., CODEN: BSCFAS, <1967>, 1175  
29. Fukui; Ohkubo, Bull.Chem.Soc.Jpn., CODEN: BCSJA8, 42, <1969>, 312  
30. Kropf et al., C.R.Seances Acad.Sci.Ser.D, CODEN: CHDDAT, <1968>, 5527

Reaction:

RX

Reaction ID: 7067053  
Reactant BRN: 3587191, 2037554, 1855036  
Reactant: hydrogen peroxide, sodium hydrogencarbonate,  
sulfuric acid, (.alpha.-chloro-isopropyl)-  
benzene  
Product BRN: 1908117, 969405  
Product: 1-methyl-1-phenyl-ethyl hydroperoxide,  
isopropenylbenzene  
No. of Reaction Details: 1

Reaction Details:

RX

Reaction RID: 7067053.1  
Reaction Classification: Chemical behaviour  
Note(s): Handbook  
Reference(s):  
1. Ross; Huettel, Chem.Ber., CODEN: CHBEAM, 89, <1956>, 2641, 2643

Reaction:

RX

Reaction ID: 6731166  
Reactant BRN: 1236613  
Reactant: isopropylbenzene  
Product BRN: 5508788, 1908117, 605842, 1905012  
Product: cumyl hydrotrioxide, 1-methyl-1-phenyl-ethyl  
hydroperoxide, 1-phenyl-ethanone,  
2-phenyl-propan-2-ol, ring product  
No. of Reaction Details: 1

Reaction Details:

RX

Reaction RID: 6731166.1  
Reaction Classification: Chemical behaviour  
Reagent: O3, O2  
Solvent: acetone-d6  
Time: 4 hour(s)  
Temperature: -40 Cel  
Other Conditions: further periods of time  
Subject Studied: Product distribution  
Reference(s):  
1. Pryor, William A.; Ohto, Norio; Church, Daniel F., J.Amer.Chem.Soc.,  
CODEN: JACSAT, 105(11), <1983>, 3614-3622; BABS-5737674

Reaction:

RX

Reaction ID: 6725969  
Reactant BRN: 1236613  
Reactant: isopropylbenzene  
Product BRN: 1908117, 1905012, 605842, 969616, 635680,  
969405  
Product: 1-methyl-1-phenyl-ethyl hydroperoxide,  
2-phenyl-propan-2-ol, 1-phenyl-ethanone,  
phenol, propan-2-one, isopropenylbenzene,  
acetic acid  
No. of Reaction Details: 1

Reaction Details:

RX

Reaction RID: 6725969.1  
Reaction Classification: Chemical behaviour  
Reagent: (t-BuO)3Al, t-BuOOH  
Solvent: benzene  
Time: 3.5 day(s)

Temperature: 20 Cel  
Subject Studied: Mechanism, Product distribution  
Reference(s):  
1. Stepovik, L. P.; Dodonov, V. A.; Zaburdaeva, E. A., Russ.J.Gen.Chem., CODEN: RJGCEK, 67(1), <1997>, 111-115, Zh.Obshch.Khim., CODEN: ZOKHA4, 67(1), <1997>, 116-120; BABS-6099494

Reaction:

RX

Reaction ID: 6674993  
Reactant BRN: 1236613  
Reactant: oxygen, metal phthalocyaninene, isopropylbenzene  
Product BRN: 1908117  
Product: 1-methyl-1-phenyl-ethyl hydroperoxide  
No. of Reaction Details: 1

Reaction Details:

RX

Reaction RID: 6674993.1  
Reaction Classification: Chemical behaviour  
Temperature: 50 - 150 Cel  
Subject Studied: Kinetics  
Note(s): Handbook  
Reference(s):  
1. Hock; Kropf, J.Prakt.Chem., CODEN: JPCEAO, <4> 9, <1959>, 173, 175

Reaction:

RX

Reaction ID: 6674992  
Reactant BRN: 1236613  
Reactant: oxygen, lead (IV) oxide, isopropylbenzene  
Product BRN: 1908117  
Product: 1-methyl-1-phenyl-ethyl hydroperoxide  
No. of Reaction Details: 1

Reaction Details:

RX

Reaction RID: 6674992.1  
Reaction Classification: Chemical behaviour  
Temperature: 80 Cel  
Subject Studied: Kinetics  
Note(s): Handbook  
Reference(s):  
1. Hock; Kropf, J.Prakt.Chem., CODEN: JPCEAO, <4> 6, <1958>, 120

Reaction:

RX

Reaction ID: 6674991  
Reactant BRN: 1236613  
Reactant: oxygen, copper, isopropylbenzene  
Product BRN: 1908117  
Product: 1-methyl-1-phenyl-ethyl hydroperoxide  
No. of Reaction Details: 1

Reaction Details:

RX

Reaction RID: 6674991.1  
Reaction Classification: Chemical behaviour  
Temperature: 120 Cel  
Subject Studied: Kinetics  
Note(s): Handbook  
Reference(s):  
1. De Boer et al., Proc.K.Ned.Akad.Wet.Ser.B:Phys.Sci., CODEN: KNWBAA, <B>

## Reaction:

RX

Reaction ID: 6674990  
Reactant BRN: 1236613  
Reactant: oxygen, copper stearate, isopropylbenzene  
Product BRN: 1908117  
Product: 1-methyl-1-phenyl-ethyl hydroperoxide  
No. of Reaction Details: 1

## Reaction Details:

RX

Reaction RID: 6674990.1  
Reaction Classification: Chemical behaviour  
Temperature: 100 Cel  
Note(s): Handbook  
Reference(s):  
1. George; Rideal; Robertson, Proc.R.Soc.London A, CODEN: PRLAAZ, 185, <1946>, 288, 297

## Reaction:

RX

Reaction ID: 6674989  
Reactant BRN: 1236613  
Reactant: oxygen, cobalt (II)-stearate, isopropylbenzene  
Product BRN: 1908117  
Product: 1-methyl-1-phenyl-ethyl hydroperoxide  
No. of Reaction Details: 1

## Reaction Details:

RX

Reaction RID: 6674989.1  
Reaction Classification: Chemical behaviour  
Temperature: 90 Cel  
Subject Studied: Kinetics  
Note(s): Handbook  
Reference(s):  
1. Kucher, Zh.Fiz.Khim., CODEN: ZFKHA9, 33, <1959>, 617, Chem.Abstr., <1959>, 21100

## Reaction:

RX

Reaction ID: 6674988  
Reactant BRN: 1236613  
Reactant: oxygen, cobalt (III)-stearate, isopropylbenzene  
Product BRN: 1908117  
Product: 1-methyl-1-phenyl-ethyl hydroperoxide  
No. of Reaction Details: 1

## Reaction Details:

RX

Reaction RID: 6674988.1  
Reaction Classification: Chemical behaviour  
Temperature: 90 Cel  
Subject Studied: Kinetics  
Note(s): Handbook  
Reference(s):  
1. Kucher, Zh.Fiz.Khim., CODEN: ZFKHA9, 33, <1959>, 617, Chem.Abstr., <1959>, 21100

## Reaction:

RX

Reaction ID: 6674987  
Reactant BRN: 1236613  
Reactant: oxygen, barium peroxide, isopropylbenzene  
Product BRN: 1908117  
Product: 1-methyl-1-phenyl-ethyl hydroperoxide  
No. of Reaction Details: 1

Reaction Details:

RX

Reaction RID: 6674987.1  
Reaction Classification: Chemical behaviour  
Temperature: 100 - 140 Cel  
Subject Studied: Kinetics  
Note(s): Handbook  
Reference(s):  
1. Tsunoda; Matsumoto, Tokai technol. J. Japan, 17(1), <1956>, 17

Reaction:

RX

Reaction ID: 6674985  
Reactant BRN: 390030, 1236613  
Reactant: oxygen, anthraquinone, isopropylbenzene  
Product BRN: 1908117  
Product: 1-methyl-1-phenyl-ethyl hydroperoxide  
No. of Reaction Details: 1

Reaction Details:

RX

Reaction RID: 6674985.1  
Reaction Classification: Chemical behaviour  
Temperature: 15 Cel  
Subject Studied: Kinetics  
Note(s): Handbook  
Reference(s):  
1. Le Berre, Bull.Soc.Chim.Fr., CODEN: BSCFAS, <1959>, 1933

Reaction:

RX

Reaction ID: 6674984  
Reactant BRN: 1238185, 1236613  
Reactant: oxygen, benzophenone, isopropylbenzene  
Product BRN: 1908117  
Product: 1-methyl-1-phenyl-ethyl hydroperoxide  
No. of Reaction Details: 2

Reaction Details:

RX

Reaction RID: 6674984.1  
Reaction Classification: Chemical behaviour  
Temperature: 100 Cel  
Subject Studied: Kinetics  
Note(s): Handbook  
Reference(s):  
1. Le Berre, Bull.Soc.Chim.Fr., CODEN: BSCFAS, <1959>, 1933

RX

Reaction RID: 6674984.2  
Reaction Classification: Chemical behaviour  
Temperature: 15 Cel  
Subject Studied: Kinetics  
Note(s): Handbook  
Reference(s):  
1. Le Berre, Bull.Soc.Chim.Fr., CODEN: BSCFAS, <1959>, 1933

Reaction:

RX

Reaction ID: 6674983  
 Reactant BRN: 1236613  
 Reactant: oxygen, isopropylbenzene  
 Product BRN: 1908117  
 Product: 1-methyl-1-phenyl-ethyl hydroperoxide  
 No. of Reaction Details: 6

Reaction Details:

RX

Reaction RID: 6674983.1  
 Reaction Classification: Chemical behaviour  
 Temperature: 90 Cel  
 Subject Studied: Kinetics  
 Note(s): Handbook  
 Reference(s):  
 1. Kucher et al., Kolloidn.Zh., CODEN: KOZHAG, 21, <1959>, 309; engl. Ausg. S. 295

RX

Reaction RID: 6674983.2  
 Reaction Classification: Chemical behaviour  
 Temperature: 60 - 120 Cel  
 Pressure: 20 - 60 Torr  
 Subject Studied: Kinetics  
 Note(s): Handbook  
 Pressure: 60 Torr  
 Reference(s):  
 1. Takahashi, Kogyo Kagaku Zasshi, CODEN: KGKZA7, 57, <1954>, 363, Chem.Abstr., <1955>, 15789

RX

Reaction RID: 6674983.3  
 Reaction Classification: Chemical behaviour  
 Temperature: 100 Cel  
 Subject Studied: Kinetics  
 Note(s): Handbook  
 Reference(s):  
 1. Le Berre, Bull.Soc.Chim.Fr., CODEN: BSCFAS, <1959>, 1933

RX

Reaction RID: 6674983.4  
 Reaction Classification: Chemical behaviour  
 Temperature: 100 - 140 Cel  
 Subject Studied: Kinetics  
 Note(s): Handbook  
 Reference(s):  
 1. Tsunoda; Matsumoto, Tokai technol. J. Japan, 17(1), <1956>, 17

RX

Reaction RID: 6674983.5  
 Reaction Classification: Chemical behaviour  
 Temperature: 120 Cel  
 Subject Studied: Kinetics  
 Note(s): Handbook  
 Reference(s):  
 1. De Boer et al., Proc.K.Ned.Akad.Wet.Ser.B:Phys.Sci., CODEN: KNWBAA, <B> 61, <1958>, 170

RX

Reaction RID: 6674983.6  
 Reaction Classification: Chemical behaviour  
 Other Conditions: UV-Licht  
 Note(s): Handbook  
 Reference(s):  
 1. Hock; Lang, Chem.Ber., CODEN: CHBEAM, 77/79, <1944/1946>, 257, 261

Reaction:



RX

Reaction ID: 5093407  
Reactant BRN: 1910303, 1923953  
Reactant: (1-methyl-1-phenyl-ethyl)-peroxyl,  
Tris-(trimethylsilyl)-silan  
Product BRN: 1908117, 2040481  
Product: 1-methyl-1-phenyl-ethyl hydroperoxide,  
Tris-(trimethyl)-silyl  
No. of Reaction Details: 1

Reaction Details:

RX

Reaction RID: 5093407.1  
Reaction Classification: Chemical behaviour  
Temperature: 72.5 Cel  
Other Conditions: also with Bu<sub>3</sub>SnH  
Subject Studied: Rate constant  
Reference(s):  
1. Chatgililoglu, Chrysostomos; Timokhin, Vitaliy I.; Zaborovskiy,  
Andriy B.; Lutsyk, Daria S.; Prystansky, Ruslan E., Chem.Comm.,  
CODEN: CHCOFS(5), <1999>, 405 - 406; BABS-6163466

Reaction:

RX

Reaction ID: 5045464  
Reactant BRN: 969405  
Reactant: isopropenylbenzene  
Product BRN: 1908117  
Product: 1-methyl-1-phenyl-ethyl hydroperoxide  
No. of Reaction Details: 1

Reaction Details:

RX

Reaction RID: 5045464.1  
Reaction Classification: Preparation  
Yield: 72 percent (BRN=1908117)  
Reagent: O<sub>2</sub>, Et<sub>3</sub>SiH  
Catalyst: Co(II) (tdcpp)  
Solvent: CH<sub>2</sub>Cl<sub>2</sub>, propan-2-ol  
Time: 1 hour(s)  
Temperature: 28 Cel  
Pressure: 760 Torr  
Reference(s):  
1. Sugamoto, Kazuhiro; Matsushita, Yoh-ichi; Matsui, Takanao,  
J.Chem.Soc.Perkin Trans.1, CODEN: JCPRB4(23), <1998>, 3989-3998;  
BABS-6130087

Reaction:

RX

Reaction ID: 4495179  
Reactant BRN: 7494642  
Reactant: C<sub>9</sub>H<sub>12</sub>\*O<sub>3</sub>  
Product BRN: 5508788, 1908117, 1905012, 605842  
Product: cumyl hydrotrioxide, 1-methyl-1-phenyl-ethyl  
hydroperoxide, 2-phenyl-propan-2-ol,  
1-phenyl-ethanone  
No. of Reaction Details: 1

Reaction Details:

RX

Reaction RID: 4495179.1  
Reaction Classification: Chemical behaviour  
Reagent: cumene  
Solvent: CH<sub>2</sub>Cl<sub>2</sub>

Temperature: -30 Cel  
Other Conditions: other temperatures; activation parameters A', A0, .delta.S0<\*>, A1; decomposition of ozone complexes with arenes; spectrophotometric study of kinetic regularities; possible mechanism of conversion of ozone complexes  
Subject Studied: Rate constant, Thermodynamic data, Kinetics  
Reference(s):  
1. Avzyanova, E. V.; Kabal'nova, N. N.; Shereshovets, V. V.,  
Russ.Chem.Bl., CODEN: RCBUEY, 45(2), <1996>, 356-359, Izv.Akad.Nauk  
Ser.Khim., CODEN: IASKEA(2), <1996>, 371-374; BABS-6013599

Reaction:

RX

Reaction ID: 4476259  
Reactant BRN: 393006, 1098229, 3610848  
Reactant: 2,3,5,6-tetrachloro-<1,4>benzoquinone, methanol, 4-methoxybicumene  
Product BRN: 6977835, 1905012, 1908117, 1859781, 3604540  
Product: 2,3,5,6-tetrachloro-4-(1-methyl-1-phenyl-ethoxy)-phenol, 2-phenyl-propan-2-ol, 1-methyl-1-phenyl-ethyl hydroperoxide, methyl-(1-methyl-1-phenyl-ethyl)-ether, 2-methoxy-2-(4'-methoxyphenyl)propane  
No. of Reaction Details: 1

Reaction Details:

RX

Reaction RID: 4476259.1  
Reaction Classification: Chemical behaviour  
Yield: 7 percent Spectr. (BRN=6977835), 7 percent Spectr. (BRN=1905012), 41 percent Spectr. (BRN=1908117), 14 percent Spectr. (BRN=1859781), 71 percent Spectr. (BRN=3604540)  
Reagent: O2  
Solvent: tetrahydrofuran-d8  
Other Conditions: Ambient temperature, Irradiation, electron transfer and fragmentation reactions of photogenerated methoxybicumene radical cations; effect of oxygen; back electron transfer in triplet ion pairs; formation of charge-transfer complexes between quinones and methoxybicumenes  
Subject Studied: Quantum yield, Rate constant, Product distribution  
Reference(s):  
1. Maslak, Przemyslaw; Chapman, William H., J.Org.Chem., CODEN: JOCEAH, 61(8), <1996>, 2647-2656; BABS-6013063

Reaction:

RX

Reaction ID: 4344720  
Reactant BRN: 2054290  
Reactant: peroxybenzoic acid-(1-methyl-1-phenyl-ethyl ester)  
Product BRN: 1908117  
Product: 1-methyl-1-phenyl-ethyl hydroperoxide  
No. of Reaction Details: 1

Reaction Details:

RX

Reaction RID: 4344720.1

Reaction Classification: Preparation  
Reagent: aq. LiOH  
Solvent: tetrahydrofuran  
Reference(s):  
1. Caldwell, Sarah E.; Porter, Ned. A., J.Amer.Chem.Soc., CODEN: JACSAT, 117(33), <1995>, 8676-8677; BABS-6002112

Reaction:

RX

Reaction ID: 3117018  
Reactant BRN: 5508788  
Reactant: cumyl hydrotrioxide  
Product BRN: 1236613, 1905012, 1908117, 605842  
Product: isopropylbenzene, 2-phenyl-propan-2-ol, 1-methyl-1-phenyl-ethyl hydroperoxide, 1-phenyl-ethanone  
No. of Reaction Details: 1

Reaction Details:

RX

Reaction RID: 3117018.1  
Reaction Classification: Chemical behaviour  
Reagent: 2,6-di-tert-butyl-4-methylphenol  
Solvent: acetone-d6  
Temperature: -18 Cel  
Other Conditions: Arrhenius parameters; other temperatures, reagents ratio  
Subject Studied: Rate constant, Thermodynamic data, Mechanism  
Reference(s):  
1. Pryor, William A.; Ohto, Norio; Church, Daniel F., J.Amer.Chem.Soc., CODEN: JACSAT, 104(21), <1982>, 5813-5814; BABS-5693890

Reaction:

RX

Reaction ID: 3090813  
Reactant BRN: 5430954  
Reactant: <1-(1-methoxy-1-methyl-ethylperoxy)-1-methyl-ethyl>-benzene  
Product BRN: 1908117  
Product: 1-methyl-1-phenyl-ethyl hydroperoxide  
No. of Reaction Details: 1

Reaction Details:

RX

Reaction RID: 3090813.1  
Reaction Classification: Preparation  
Reagent: AcOH, H2O  
Solvent: tetrahydrofuran  
Time: 24 hour(s)  
Note(s): Yield given  
Reference(s):  
1. Bloodworth, A. J.; Cooksey, Christhopher J.; Korkodilos, Despoina, J.Chem.Soc.Chem.Comm., CODEN: JCCCCAT(13), <1992>, 926-927; BABS-5656223

Reaction:

RX

Reaction ID: 2297353  
Reactant BRN: 3610848  
Reactant: 4-methoxybicumene  
Product BRN: 3604540, 1908117, 1905012  
Product: 2-methoxy-2-(4'-methoxyphenyl)propane, 1-methyl-1-phenyl-ethyl hydroperoxide, 2-phenyl-propan-2-ol

No. of Reaction Details: 2

Reaction Details:

RX

Reaction RID: 2297353.1  
Reaction Classification: Preparation  
Yield: 100 percent Spectr. (BRN=3604540), 20 percent Spectr. (BRN=1908117), 78 percent Spectr (BRN=1905012)  
Reagent: 1,4-dicyanobenzene, O2  
Solvent: tetrahydrofuran, methanol  
Temperature: 22 Cel  
Other Conditions: Irradiation  
Reference(s):  
1. Maslak, Przemyslaw; Chapman, William H., Tetrahedron, CODEN: TETRAB, 46(8), <1990>, 2715-2724; BABS-5511977

RX

Reaction RID: 2297353.2  
Reaction Classification: Preparation  
Yield: 100 percent Spectr. (BRN=3604540), 78 percent Spectr. (BRN=1905012), 20 percent Spectr (BRN=1908117)  
Reagent: 1,4-dicyanobenzene, O2  
Solvent: tetrahydrofuran, methanol  
Temperature: 22 Cel  
Other Conditions: Irradiation  
Reference(s):  
1. Maslak, Przemyslaw; Chapman, William H., Tetrahedron, CODEN: TETRAB, 46(8), <1990>, 2715-2724; BABS-5511977

Reaction:

RX

Reaction ID: 2297352  
Reactant BRN: 3610848  
Reactant: 4-methoxybicumene  
Product BRN: 1908117, 1905012  
Product: 1-methyl-1-phenyl-ethyl hydroperoxide, 2-phenyl-propan-2-ol  
No. of Reaction Details: 1

Reaction Details:

RX

Reaction RID: 2297352.1  
Reaction Classification: Preparation  
Reagent: oxygen  
Other Conditions: Irradiation  
Reference(s):  
1. Maslak, Przemyslaw; Chapman, Jr. William H., J.Chem.Soc.Chem.Comm., CODEN: JCCCAT(23), <1989>, 1809-1811; BABS-5918901  
2. Maslak, Przemyslaw; Chapman, Jr. William H., J.Chem.Soc.Chem.Comm., CODEN: JCCCAT(23), <1989>, 1809-1811; BABS-5918901

Reaction:

RX

Reaction ID: 2020496  
Reactant BRN: 1910303  
Reactant: (1-methyl-1-phenyl-ethyl)-peroxyl  
Product BRN: 1908117  
Product: 1-methyl-1-phenyl-ethyl hydroperoxide  
No. of Reaction Details: 3

Reaction Details:

RX

Reaction RID: 2020496.1

Reaction Classification: Chemical behaviour  
Reagent: tBuSi(H)Me<sub>2</sub>  
Temperature: 72.35 Cel  
Subject Studied: Kinetics  
Reaction Type: Reduction  
Prototype Reaction: Further Variations:, Reagents  
Reference(s):  
1. Chatgililoglu, Chrysostomos; Timokhin, Vitaliy I.; Zaborovskiy, Andriy B.; Lutsyk, Daria S.; Prystansky, Ruslan E., J.Chem.Soc.Perkin Trans.2, CODEN: JCPKBH(3), <2000>, 577 - 582; BABS-6238109

RX

Reaction RID: 2020496.2  
Reaction Classification: Chemical behaviour  
Reagent: diphenylamine, O<sub>2</sub>, AIBN  
Solvent: chlorobenzene  
Temperature: 348.5 Cel  
Subject Studied: Rate constant  
Reference(s):  
1. Varlamov, V. T.; Denisov, E. T., Bull.Acad.Sci.USSR Div.Chem.Sci.(Engl.Transl.), CODEN: BACCAT, 36(8), <1987>, 1607-1612, Izv.Akad.Nauk SSSR Ser.Khim., CODEN: IASKA6(8), <1987>, 1738-1743; BABS-5740678

RX

Reaction RID: 2020496.3  
Reaction Classification: Chemical behaviour  
Reagent: <meso-tetrakis(2,6-dimethyl-3-sulfonatophenyl)porphinato>manganese(III) hydrate, NaNO<sub>3</sub>, buffer pH 10 (HCO<sub>3</sub><sup>-</sup>/CO<sub>3</sub><sup>2-</sup>), H<sub>2</sub>O<sub>2</sub>, air  
Temperature: 30 Cel  
Subject Studied: Rate constant, Equilibrium constant, Mechanism  
Reference(s):  
1. Arasasingham, Ramesh D.; Jeon, Seungwon; Bruce, Thomas C., J.Amer.Chem.Soc., CODEN: JACSAT, 114(7), <1992>, 2536-2544; BABS-5647883

Reaction:

RX

Reaction ID: 2020495  
Reactant BRN: 1910303, 2384864  
Reactant: (1-methyl-1-phenyl-ethyl)-peroxyl, hexahydroxy-<1,4>naphthoquinone  
Product BRN: 1908117  
Product: 1-methyl-1-phenyl-ethyl hydroperoxide  
No. of Reaction Details: 1

Reaction Details:

RX

Reaction RID: 2020495.1  
Reaction Classification: Chemical behaviour  
Temperature: 60 Cel  
Subject Studied: Rate constant  
Reference(s):  
1. Boguslavskaya, L. V.; Khrapova, N. G.; Maksimov, O. B., Bull.Acad.Sci.USSR Div.Chem.Sci.(Engl.Transl.), CODEN: BACCAT, 34(7), <1985>, 1345-1350, Izv.Akad.Nauk SSSR Ser.Khim., CODEN: IASKA6(7), <1985>, 1471-1476; BABS-5798349

Reaction:

RX

Reaction ID: 2020494  
Reactant BRN: 1910303, 2147084  
Reactant: (1-methyl-1-phenyl-ethyl)-peroxyl,

6-ethyl-2,3,5,7,8-pentahydroxy-  
<1,4>naphthoquinone  
Product BRN: 1908117  
Product: 1-methyl-1-phenyl-ethyl hydroperoxide  
No. of Reaction Details: 1

Reaction Details:

RX

Reaction RID: 2020494.1  
Reaction Classification: Chemical behaviour  
Temperature: 60 Cel  
Subject Studied: Rate constant  
Reference(s):  
1. Boguslavskaya, L. V.; Khrapova, N. G.; Maksimov, O. B.,  
Bull.Acad.Sci.USSR Div.Chem.Sci.(Engl.Transl.), CODEN: BACCAT, 34(7),  
<1985>, 1345-1350, Izv.Akad.Nauk SSSR Ser.Khim., CODEN: IASKA6(7),  
<1985>, 1471-1476; BABS-5798349

Reaction:

RX

Reaction ID: 2020493  
Reactant BRN: 1910303, 2146863  
Reactant: (1-methyl-1-phenyl-ethyl)-peroxyl,  
2-acetyl-3,5,6,8-tetrahydroxy-  
<1,4>naphthoquinone  
Product BRN: 1908117  
Product: 1-methyl-1-phenyl-ethyl hydroperoxide  
No. of Reaction Details: 1

Reaction Details:

RX

Reaction RID: 2020493.1  
Reaction Classification: Chemical behaviour  
Temperature: 60 Cel  
Subject Studied: Rate constant  
Reference(s):  
1. Boguslavskaya, L. V.; Khrapova, N. G.; Maksimov, O. B.,  
Bull.Acad.Sci.USSR Div.Chem.Sci.(Engl.Transl.), CODEN: BACCAT, 34(7),  
<1985>, 1345-1350, Izv.Akad.Nauk SSSR Ser.Khim., CODEN: IASKA6(7),  
<1985>, 1471-1476; BABS-5798349

Reaction:

RX

Reaction ID: 2020492  
Reactant BRN: 1910303, 2131494  
Reactant: (1-methyl-1-phenyl-ethyl)-peroxyl,  
2,3,5,6,8(oder 2,5,6,7,8)-pentahydroxy-  
<1,4>naphthoquinone  
Product BRN: 1908117  
Product: 1-methyl-1-phenyl-ethyl hydroperoxide  
No. of Reaction Details: 1

Reaction Details:

RX

Reaction RID: 2020492.1  
Reaction Classification: Chemical behaviour  
Temperature: 60 Cel  
Subject Studied: Rate constant  
Reference(s):  
1. Boguslavskaya, L. V.; Khrapova, N. G.; Maksimov, O. B.,  
Bull.Acad.Sci.USSR Div.Chem.Sci.(Engl.Transl.), CODEN: BACCAT, 34(7),  
<1985>, 1345-1350, Izv.Akad.Nauk SSSR Ser.Khim., CODEN: IASKA6(7),  
<1985>, 1471-1476; BABS-5798349

## Reaction:

RX

Reaction ID: 2020491  
Reactant BRN: 1910303, 2003780  
Reactant: (1-methyl-1-phenyl-ethyl)-peroxyl,  
2-acetyl-3,5,6,7,8-pentahydroxy-  
<1,4>naphthoquinone  
Product BRN: 1908117  
Product: 1-methyl-1-phenyl-ethyl hydroperoxide  
No. of Reaction Details: 1

## Reaction Details:

RX

Reaction RID: 2020491.1  
Reaction Classification: Chemical behaviour  
Temperature: 60 Cel  
Subject Studied: Rate constant  
Reference(s):  
1. Boguslavskaya, L. V.; Khrapova, N. G.; Maksimov, O. B.,  
Bull.Acad.Sci.USSR Div.Chem.Sci.(Engl.Transl.), CODEN: BACCAT, 34(7),  
<1985>, 1345-1350, Izv.Akad.Nauk SSSR Ser.Khim., CODEN: IASKA6(7),  
<1985>, 1471-1476; BABS-5798349

## Reaction:

RX

Reaction ID: 1709985  
Reactant BRN: 1236613  
Reactant: isopropylbenzene  
Product BRN: 1908117, 605842, 969616, 2056090  
Product: 1-methyl-1-phenyl-ethyl hydroperoxide,  
2-phenyl-propan-2-ol, 1-phenyl-ethanone,  
phenol, bis-(1-methyl-1-phenyl-ethyl)-  
peroxide  
No. of Reaction Details: 2

## Reaction Details:

RX

Reaction RID: 1709985.1  
Reaction Classification: Chemical behaviour  
Yield: 88.8 percent (BRN=1908117)  
Reagent: O2, AlCl-phthalocyanine  
Time: 1.1 hour(s)  
Temperature: 130 Cel  
Other Conditions: mechanism; other times and temperatures;  
other phthalocyanine; further reagent;  
various concentrations of reagent;  
activation energies  
Subject Studied: Kinetics, Thermodynamic data, Product  
distribution  
Reference(s):  
1. Kropf, Heinz; Vogel, Werner, J.Chem.Res.Miniprint, CODEN: JRMPDM(1),  
<1986>, 0315-0342; BABS-5867413

RX

Reaction RID: 1709985.2  
Reaction Classification: Chemical behaviour  
Yield: 92.8 percent (BRN=1908117)  
Reagent: O2, Sn(OH)2-phthalocyanine  
Time: 5.7 hour(s)  
Temperature: 110 Cel  
Other Conditions: mechanism; other times and temperatures;  
other phthalocyanines; various  
concentrations of reagent; activation  
energies  
Subject Studied: Kinetics, Thermodynamic data, Product

## distribution

## Reference(s):

1. Kropf, Heinz; Vogel, Werner; Hopf, Christiane, J.Chem.Res.Miniprint, CODEN: JRMPDM(1), <1986>, 0301-0314; BABS-5867412

## Reaction:

RX

Reaction ID: 1709984  
Reactant BRN: 1236613  
Reactant: isopropylbenzene  
Product BRN: 1908117, 605842, 1905012, 969405, 969616  
Product: 1-methyl-1-phenyl-ethyl hydroperoxide,  
1-phenyl-ethanone, 2-phenyl-propan-2-ol,  
isopropenylbenzene, phenol  
No. of Reaction Details: 2

## Reaction Details:

RX

Reaction RID: 1709984.1  
Reaction Classification: Chemical behaviour  
Reagent: O2  
Catalyst: zinc naphthenate-1,10-phenanthroline  
Time: 8 hour(s)  
Temperature: 100 Cel  
Other Conditions: rate constants between 100-130 deg C  
Subject Studied: Kinetics, Product distribution  
Reference(s):  
1. Kozlov, S. K.; Tovstokhat'ko, F. I.; Potekhin, V. M., J.Appl.Chem.USSR (Engl.Transl.), CODEN: JAPUAW, 59, <1986>, 1284-1286, Zh.Prikl.Khim.(Leningrad), CODEN: ZPKHAB, 59(6), <1986>, 1378-1380; BABS-5877997

RX

Reaction RID: 1709984.2  
Reaction Classification: Chemical behaviour  
Reagent: O2  
Catalyst: 1.5E-4 zinc naphthenate  
Time: 3 hour(s)  
Temperature: 110 Cel  
Other Conditions: activation energy; different catalyst, catalyst concentrations, reaction times and temperatures  
Subject Studied: Product distribution, Kinetics, Thermodynamic data  
Reference(s):  
1. Kozlov, S. K.; Tovstokhat'ko, F. I.; Potekhin, V. M., J.Appl.Chem.USSR (Engl.Transl.), CODEN: JAPUAW, 59, <1986>, 122-127, Zh.Prikl.Khim.(Leningrad), CODEN: ZPKHAB, 59(1), <1986>, 134-139; BABS-5875963

## Reaction:

RX

Reaction ID: 1709981  
Reactant BRN: 1236613  
Reactant: isopropylbenzene  
Product BRN: 605842, 1908117  
Product: 1-phenyl-ethanone, 1-methyl-1-phenyl-ethyl hydroperoxide  
No. of Reaction Details: 1

## Reaction Details:

RX

Reaction RID: 1709981.1  
Reaction Classification: Chemical behaviour  
Catalyst: <ZnNf2>/o-phenanthroline



Time: 6 hour(s)  
Temperature: 110 Cel  
Other Conditions: depedence of the initial rate of oxidation  
on the catalyst-activator ratio; effect of  
various catalysts; influence of the catalyst  
concentration on the selectivity for CHP  
Subject Studied: Product distribution

Reference(s):

1. Kozlov, S. K.; Tovstokhat'ko, F. I.; Potekhin, V. M., J.Appl.Chem.USSR  
(Engl.Transl.), CODEN: JAPUAW, 59(5), <1986>, 1061-1063,  
Zh.Prikl.Khim.(Leningrad), CODEN: ZPKHAB, 59(5), <1986>, 1138-1140;  
BABS-5881749

Reaction:

RX

Reaction ID: 1709979  
Reactant BRN: 1236613  
Reactant: isopropylbenzene  
Product BRN: 1905012, 1908117, 605842, 5508788  
Product: 2-phenyl-propan-2-ol, 1-methyl-1-phenyl-  
ethyl hydroperoxide, 1-phenyl-ethanone,  
cumyl hydrotrioxide  
No. of Reaction Details: 1

Reaction Details:

RX

Reaction RID: 1709979.1  
Reaction Classification: Preparation  
Yield: 2 percent (BRN=5508788)  
Reagent: ozone  
Solvent: acetone-d6  
Time: 3 hour(s)  
Temperature: -40 Cel  
Note(s): Yields of byproduct given  
Reference(s):  
1. Pryor, William A.; Ohto, Norio; Church, Daniel F., J.Amer.Chem.Soc.,  
CODEN: JACSAT, 104(21), <1982>, 5813-5814; BABS-5693890

Reaction:

RX

Reaction ID: 1709978  
Reactant BRN: 1236613  
Reactant: isopropylbenzene  
Product BRN: 1908117, 1905012, 605842, 2056090  
Product: 1-methyl-1-phenyl-ethyl hydroperoxide,  
2-phenyl-propan-2-ol, 1-phenyl-ethanone,  
bis-(1-methyl-1-phenyl-ethyl)-peroxide  
No. of Reaction Details: 1

Reaction Details:

RX

Reaction RID: 1709978.1  
Reaction Classification: Chemical behaviour  
Yield: 0.36 mol (BRN=1908117), 0.035 mol  
(BRN=1905012), 0.0014 mol (BRN=605842),  
0.0015 mol (BRN=2056090)  
Reagent: 2,2,3,3-tetraphenylbutane, O2  
Time: 48 hour(s)  
Temperature: 29.9 Cel  
Pressure: 304 Torr  
Other Conditions: variation of reagent, pressure, reaction  
time  
Subject Studied: Rate constant, Product distribution  
Reference(s):

1. Howard, J. A.; Bennett, J. E.; Brunton, G., Can.J.Chem., CODEN: CJCHAG, 59, <1981>, 2253-2260; BABS-5663809

Reaction:

RX

Reaction ID: 1709977  
Reactant BRN: 1236613  
Reactant: isopropylbenzene  
Product BRN: 1905012, 1908117, 605842  
Product: 2-phenyl-propan-2-ol, 1-methyl-1-phenyl-ethyl hydroperoxide, 1-phenyl-ethanone  
No. of Reaction Details: 5

Reaction Details:

RX

Reaction RID: 1709977.1  
Reaction Classification: Preparation  
Yield: 14 percent Spectr. (BRN=1905012), 8 percent Spectr. (BRN=1908117), 9 percent Spectr (BRN=605842)  
Reagent: dioxygen  
Catalyst: cerium (IV) ammonium nitrate,  
Solvent: acetonitrile  
Time: 5 hour(s)  
Other Conditions: Ambient temperature, Irradiation  
Note(s): Title compound not separated from byproducts  
Reference(s):  
1. Baciocchi, E.; Giacco, T. Del; Sebastiani, G. V.; Rol, C., Tetrahedron Lett., CODEN: TELEAY, 26(28), <1985>, 3353-3356; BABS-5552479

RX

Reaction RID: 1709977.2  
Reaction Classification: Preparation  
Yield: 9 percent Spectr. (BRN=605842), 8 percent Spectr. (BRN=1908117), 14 percent Spectr (BRN=1905012)  
Reagent: dioxygen  
Catalyst: cerium (IV) ammonium nitrate,  
Solvent: acetonitrile  
Time: 5 hour(s)  
Other Conditions: Ambient temperature, Irradiation  
Note(s): Title compound not separated from byproducts  
Reference(s):  
1. Baciocchi, E.; Giacco, T. Del; Sebastiani, G. V.; Rol, C., Tetrahedron Lett., CODEN: TELEAY, 26(28), <1985>, 3353-3356; BABS-5552479

RX

Reaction RID: 1709977.3  
Reaction Classification: Chemical behaviour  
Reagent: O2  
Catalyst: 1.5E-4 M MgNf2, 6E-4 M Phen  
Time: 4 hour(s)  
Temperature: 110 Cel  
Other Conditions: different catalytic systems and reaction times  
Subject Studied: Product distribution  
Reference(s):  
1. Kozlov, S. K.; Tovstokhat'ko, F. I.; Potekhin, V. M., J.Appl.Chem.USSR (Engl.Transl.), CODEN: JAPUAW, 59, <1986>, 205-207, Zh.Prikl.Khim.(Leningrad), CODEN: ZPKHAB, 59(1), <1986>, 217-219; BABS-5876061

RX

Reaction RID: 1709977.4  
Reaction Classification: Preparation  
Yield: 9 percent Spectr. (BRN=605842), 14 percent Spectr. (BRN=1905012), 8 percent Spectr

(BRN=1908117)  
Reagent: dioxygen  
Catalyst: cerium (IV) ammonium nitrate,  
Solvent: acetonitrile  
Time: 5 hour(s)  
Other Conditions: Ambient temperature, Irradiation  
Note(s): Title compound not separated from byproducts  
Reference(s):  
1. Baciocchi, E.; Giacco, T. Del; Sebastiani, G. V.; Rol, C., Tetrahedron Lett., CODEN: TELEAY, 26(28), <1985>, 3353-3356; BABS-5552479

RX

Reaction RID: 1709977.5  
Reaction Classification: Chemical behaviour  
Yield: 38.0 percent (BRN=1908117), 0.28 percent (BRN=605842), 2.24 percent (BRN=1905012)  
Reagent: O2  
Catalyst: zinc pyrazolonate, 1,10-phenanthroline  
Time: 5.0 hour(s)  
Temperature: 110 Cel  
Other Conditions: effect of further monodentate and bidentate activators  
Subject Studied: Product distribution  
Reference(s):  
1. Kozlov, S. K.; Tovstokhat'ko, F. I.; Potekhin, V. M., J.Appl.Chem.USSR (Engl.Transl.), CODEN: JAPUAW, 59, <1986>, 1287-1290, Zh.Prikl.Khim.(Leningrad), CODEN: ZPKHAB, 59(6), <1986>, 1381-1384; BABS-5877998

Reaction:

RX

Reaction ID: 278976  
Reactant BRN: 1905012  
Reactant: 2-phenyl-propan-2-ol  
Product BRN: 1908117  
Product: 1-methyl-1-phenyl-ethyl hydroperoxide  
No. of Reaction Details: 1

Reaction Details:

RX

Reaction RID: 278976.1  
Reaction Classification: Preparation  
Reagent: aqueous H2O2, H2SO4  
Note(s): Handbook  
Reference(s):  
1. Ross; Huettel, Chem.Ber., CODEN: CHBEAM, 89, <1956>, 2641

Reaction:

RX

Reaction ID: 267155  
Reactant BRN: 1855036  
Reactant: (.alpha.-chloro-isopropyl)-benzene  
Product BRN: 1908117  
Product: 1-methyl-1-phenyl-ethyl hydroperoxide  
No. of Reaction Details: 1

Reaction Details:

RX

Reaction RID: 267155.1  
Reaction Classification: Preparation  
Reagent: aqueous H2O2, NaHCO3, H2SO4  
Note(s): Handbook  
Reference(s):  
1. Ross; Huettel, Chem.Ber., CODEN: CHBEAM, 89, <1956>, 2641

Reaction:

RX

Reaction ID: 108026  
 Reactant BRN: 1236613  
 Reactant: isopropylbenzene  
 Product BRN: 1908117  
 Product: 1-methyl-1-phenyl-ethyl hydroperoxide  
 No. of Reaction Details: 36

Reaction Details:

RX

Reaction RID: 108026.1  
 Reaction Classification: Preparation  
 Reagent: steam, oxygen  
 Note(s): Handbook  
 Reference(s):  
 1. Patent: Distillers Co. DE 819092 1949, DRP/DRBP Org.Chem.

RX

Reaction RID: 108026.2  
 Reaction Classification: Preparation  
 Reagent: anthraquinone, oxygen  
 Other Conditions: Irradiation.UV-Belichtung  
 Note(s): Handbook  
 Reference(s):  
 1. Le Berre, Bull.Soc.Chim.Fr., CODEN: BSCFAS, <1959>, 1933, 1935

RX

Reaction RID: 108026.3  
 Reaction Classification: Preparation  
 Reagent: terephthalic acid, oxygen  
 Note(s): Handbook  
 Reference(s):  
 1. Patent: Montecatini US 2799711 1956

RX

Reaction RID: 108026.4  
 Reaction Classification: Preparation  
 Reagent: acetoacetic acid ethyl ester, oxygen  
 Note(s): Handbook  
 Reference(s):  
 1. Patent: Soc. Usines Chim. Rhone-Poulenc US 2674629 1953

RX

Reaction RID: 108026.5  
 Reaction Classification: Preparation  
 Reagent: cerium naphthenate, oxygen  
 Note(s): Handbook  
 Reference(s):  
 1. Patent: Farbenfabr. Bayer US 2655545 1951  
 2. Patent: Farbenfabr. Bayer DE 889443 1951, DRP/DRBP Org.Chem.  
 3. Patent: Farbenfabr. Bayer DE 969744 1950

RX

Reaction RID: 108026.6  
 Reaction Classification: Preparation  
 Reagent: oxygen  
 Temperature: 85 Cel  
 Other Conditions: UV-Licht  
 Note(s): Handbook  
 Reference(s):  
 1. George; Rideal; Robertson, Proc.R.Soc.London A, CODEN: PRLAAZ, 185, <1946>, 288, 292, 297  
 2. Hock; Lang, Chem.Ber., CODEN: CHBEAM, 77/79, <1944/1946>, 257, 261

RX

Reaction RID: 108026.7  
 Reaction Classification: Preparation  
 Reagent: Na2CO3, oxygen  
 Note(s): Handbook

Reference(s):

1. Patent: Allied Chem. & Dye Corp. US 2629744 1950
2. Patent: Allied Chem. & Dye Corp. US 2681936 1950

RX

Reaction RID: 108026.8  
Reaction Classification: Preparation  
Reagent: aqueous sodium stearate, oxygen  
Note(s): Handbook

Reference(s):

1. Armstrong et al., J.Chem.Soc., CODEN: JCSOA9, <1950>, 666
2. Patent: Hercules Powder Co. US 2547938 1947

RX

Reaction RID: 108026.9  
Reaction Classification: Chemical behaviour  
Yield: 18 percent Chromat. (BRN=1908117)  
Reagent: 102, 9-diazofluorene, meso-tetraphenylporphine  
Solvent: benzene  
Time: 30 min  
Temperature: 20 Cel  
Other Conditions: Irradiation, O-transfer reaction; trapping of carbonyl oxide from 9-diazofluorene

Subject Studied:

Product distribution, Mechanism

Reference(s):

1. Sawaki, Yasuhiko; Kato, Hiroshi; Ogata, Yoshiro, J.Amer.Chem.Soc., CODEN: JACSAT, 103(13), <1981>, 3832-3837; BABS-5691150

RX

Reaction RID: 108026.10  
Reaction Classification: Preparation  
Reagent: oxygen  
Time: 8 hour(s)  
Temperature: 110 Cel

Reference(s):

1. Kozlov, S. K.; Tovstokhat'ko, F. I.; Potekhin, V. M., J.Appl.Chem.USSR (Engl.Transl.), CODEN: JAPUAW, 58, <1985>, 2490-2494, Zh.Prikl.Khim.(Leningrad), CODEN: ZPKHAB, 58(12), <1985>, 2696-2701; BABS-5877528

RX

Reaction RID: 108026.11  
Reaction Classification: Chemical behaviour  
Reagent: p-dihydroxybenzene, azoisobutyronitrile  
Solvent: acetic acid  
Temperature: 60 Cel  
Other Conditions: other reagent, other solvent, other temperature, various concentrations of the substrate, various concentrations of the reagent

Subject Studied:

Kinetics, Rate constant

Reference(s):

1. Nikolaevskii, A.N.; Kaloerova, V.G.; Kucher, R.V., J.Org.Chem.USSR (Engl.Transl.), CODEN: JOCYA9, 17, <1981>, 510-514, Zh.Org.Khim., CODEN: ZORKAE, <1> 17(3), <1981>, 595-600; BABS-5631011

RX

Reaction RID: 108026.12  
Reaction Classification: Preparation  
Reagent: azobisisobutyronitrile  
Time: 6 hour(s)  
Temperature: 95 Cel

Reference(s):

1. Kozlov, S. K.; Tovstokhat'ko, F. I.; Potekhin, V. M., J.Appl.Chem.USSR (Engl.Transl.), CODEN: JAPUAW, 59(5), <1986>, 993-996, Zh.Prikl.Khim.(Leningrad), CODEN: ZPKHAB, 59(5), <1986>, 1072-1076; BABS-5881743

RX

Reaction RID: 108026.13  
Reaction Classification: Preparation  
Reagent: oxygen  
Note(s): Handbook  
Reference(s):  
1. Patent: Shell Devel. Co. US 2633476 1952

RX

Reaction RID: 108026.14  
Reaction Classification: Chemical behaviour  
Reagent: O<sub>2</sub>, diethyl ester of 2-chloro-2(1-cyclohexenyl)ethylenylphosphonic acid, AIBN  
Temperature: 59.9 Cel  
Other Conditions: antioxidant effect of further dialkyl esters and dialkyl thioesters of 2-chloro-2(1-cyclohexenyl)ethylenylphosphonic acid at various temperature; effect of O<sub>2</sub> partial pressure on the initiated oxidation  
Subject Studied: Mechanism  
Reference(s):  
1. Ivanov, Slavi K.; Shopova, Nicolaida St.; Angelov, Christo M., Phosphorus Sulfur, CODEN: PREEDF, 26, <1986>, 105-110; BABS-5827359

RX

Reaction RID: 108026.15  
Reaction Classification: Preparation  
Reagent: O<sub>2</sub>, azobisisobutyronitrile  
Catalyst: monophenanthrolinezinc(II) pyrazolonate  
Temperature: 75 Cel  
Pressure: 760 Torr  
Reference(s):  
1. Kozlov, S. K.; Potekhin, V. M., J.Appl.Chem.USSR (Engl.Transl.), CODEN: JAPUAW, 59(7), <1986>, 1519-1521, Zh.Prikl.Khim.(Leningrad), CODEN: ZPKHAB, 59(7), <1986>, 1633-1635; BABS-5883617

RX

Reaction RID: 108026.16  
Reaction Classification: Chemical behaviour  
Reagent: O<sub>2</sub>, 2-cyano-2-propyl hydroperoxide  
Temperature: 90 Cel  
Other Conditions: further oxidation initiators, further temperatures  
Subject Studied: Kinetics  
Reference(s):  
1. Burghardt, Aleksandra; Kulicki, Zdzislaw, Monatsh.Chem., CODEN: MOCMB7, 115, <1984>, 87-92; BABS-5796729

RX

Reaction RID: 108026.17  
Reaction Classification: Preparation  
Reagent: O<sub>2</sub>, 2-cyano-2-propyl hydroperoxide  
Reference(s):  
1. Burghardt, Aleksandra; Kulicki, Zdzislaw, Monatsh.Chem., CODEN: MOCMB7, 115, <1984>, 87-92; BABS-5796729

RX

Reaction RID: 108026.18  
Reaction Classification: Chemical behaviour  
Reagent: O<sub>2</sub>, AIBN  
Temperature: 60 Cel  
Other Conditions: further reagents, initiation rates, kinetic curves  
Reference(s):  
1. Boguslavskaya, L. V.; Khrapova, N. G.; Maksimov, O. B., Bull.Acad.Sci.USSR Div.Chem.Sci.(Engl.Transl.), CODEN: BACCAT, 34(7), <1985>, 1345-1350, Izv.Akad.Nauk SSSR Ser.Khim., CODEN: IASKA6(7), <1985>, 1471-1476; BABS-5798349

RX

Reaction RID: 108026.19

Reaction Classification: Chemical behaviour  
Reagent: O<sub>2</sub>  
Catalyst: copper(I) and copper(II) compounds  
Temperature: 70 Cel  
Other Conditions: var. pressure O<sub>2</sub>, also pyridine as reagent  
Subject Studied: Mechanism  
Reference(s):  
1. Stec, Zbigniew; Kulicki, Zdzislaw, Pol.J.Chem., CODEN: PJCHDQ, 57(7-9), <1983>, 941-945; BABS-5804264

RX

Reaction RID: 108026.20  
Reaction Classification: Chemical behaviour  
Reagent: oxygen  
Catalyst: CdNf<sub>2</sub>  
Time: 8 hour(s)  
Temperature: 110 Cel  
Other Conditions: var. catalyst  
Subject Studied: Kinetics  
Reference(s):  
1. Kozlov, S. K.; Tovstokhat'ko, F. I.; Potekhin, V. M., J.Appl.Chem.USSR (Engl.Transl.), CODEN: JAPUAW, 58, <1985>, 2490-2494, Zh.Prikl.Khim.(Leningrad), CODEN: ZPKHAB, 58(12), <1985>, 2696-2701; BABS-5877528

RX

Reaction RID: 108026.21  
Reaction Classification: Chemical behaviour  
Reagent: O<sub>2</sub>, azobisisobutyronitrile  
Catalyst: monophenanthrolinezinc(II) pyrazolonate  
Temperature: 60 - 85 Cel  
Pressure: 760 Torr  
Other Conditions: further pressures, catalyst  
Subject Studied: Mechanism, Thermodynamic data, Kinetics  
Reference(s):  
1. Kozlov, S. K.; Potekhin, V. M., J.Appl.Chem.USSR (Engl.Transl.), CODEN: JAPUAW, 59(7), <1986>, 1519-1521, Zh.Prikl.Khim.(Leningrad), CODEN: ZPKHAB, 59(7), <1986>, 1633-1635; BABS-5883617

RX

Reaction RID: 108026.22  
Reaction Classification: Chemical behaviour  
Reagent: O<sub>2</sub>  
Catalyst: Co(acac)<sub>2</sub>  
Time: 10 hour(s)  
Temperature: 60 Cel  
Other Conditions: with crown ethers; rate of oxidation  
Subject Studied: Product distribution  
Reference(s):  
1. Kochinashvili, M. V.; Kuramshin, E. M.; Kotlyar, S. A.; Zlot-skii, S. S.; Rakhmankulov, D. L., J.Appl.Chem.USSR (Engl.Transl.), CODEN: JAPUAW, 62(7.2), <1989>, 1562-1564, Zh.Prikl.Khim.(Leningrad), CODEN: ZPKHAB, 62(7), <1989>, 1681-1684; BABS-5512252

RX

Reaction RID: 108026.23  
Reaction Classification: Preparation  
Reagent: NaCl, KNO<sub>3</sub>, oxygen  
Note(s): Handbook  
Reference(s):  
1. Patent: Allied Chem. & Dye Corp. US 2776999 1952

RX

Reaction RID: 108026.24  
Reaction Classification: Chemical behaviour  
Reagent: O<sub>2</sub>  
Catalyst: different cobalt catalysts  
Subject Studied: Kinetics  
Reference(s):

1. Setinek, Karel; Drapakova, Stanislava; Prokop, Zdenek,  
Collect.Czech.Chem.Comm., CODEN: CCCCAK, 51(9), <1986>, 1958-1963;  
BABS-5561803

RX

Reaction RID: 108026.25  
Reaction Classification: Chemical behaviour  
Reagent: dioxygen, cumene hydroperoxide,  
2,4-pentanedionates of Cr(III)  
Solvent: heptane  
Temperature: 60 Cel  
Other Conditions: other radical initiator and  
2,4-pentanedionates of 3d-transition metals,  
various concentration of the reagents

Reference(s):

1. Lunak, Stanislav; Chmelikova, Ruzena; Lederer, Pavel,  
Collect.Czech.Chem.Comm., CODEN: CCCCAK, 56(2), <1991>, 344-350;  
BABS-5535278

RX

Reaction RID: 108026.26  
Reaction Classification: Chemical behaviour  
Reagent: 1,4,7,10,13,16-hexaoxacyclooctadecane  
Temperature: 60 Cel  
Other Conditions: oxidation  
Subject Studied: Rate constant

Reference(s):

1. Kochinashvili, M. V.; Kuramshin, E. M.; Zlot-skii, S. S.; Rakhmankulov,  
D. L., J.Gen.Chem.USSR (Engl.Transl.), CODEN: JGCHA4, 60(3.2), <1990>,  
574-577, Zh.Obshch.Khim., CODEN: ZOKHA4, 60(3), <1990>, 657-660;  
BABS-5537965

RX

Reaction RID: 108026.27  
Reaction Classification: Chemical behaviour  
Reagent: O2  
Catalyst: phenanthroline-pyrazolone-Zn(II)-complex  
Temperature: 110 Cel  
Other Conditions: other temperature, other catalysts,  
additives  
Subject Studied: Kinetics

Reference(s):

1. Kozlov, S. K., J.Gen.Chem.USSR (Engl.Transl.), CODEN: JGCHA4, 60(1.2),  
<1990>, 153-157, Zh.Obshch.Khim., CODEN: ZOKHA4, 60(1), <1990>,  
175-180; BABS-5531529

RX

Reaction RID: 108026.28  
Reaction Classification: Chemical behaviour  
Reagent: MeOCH2CH(SH)CH2NH(m-MePh), air,  
azoisobutyronitrile  
Solvent: chlorobenzene  
Temperature: 110 Cel  
Other Conditions: var. methoxy-substituted  
1,2-aminopropanethiols  
Subject Studied: Mechanism, Rate constant

Reference(s):

1. Farzaliyev, V. M.; Allakhverdiyev, M. A.; Rzayeva, I. A.; Akhundova, M.  
M.; Nasirova, F. N.; Guseinova, A. T., Pet.Chem.USSR (Engl.Transl.),  
CODEN: PECHAM, 34(6), <1994>, 524-529, Neftekhimiya, CODEN: NEFTAH,  
34(6), <1994>, 537-541; BABS-5971722

RX

Reaction RID: 108026.29  
Reaction Classification: Chemical behaviour  
Reagent: oxygen  
Catalyst: tetraethylammonium perchlorate  
Solvent: chlorobenzene, benzonitrile  
Time: 210 min



Temperature: 84.85 Cel  
Subject Studied: Kinetics  
Reaction Type: Oxidation  
Prototype Reaction: Further Variations:, Catalysts  
Reference(s):  
1. Opeida, I. A.; Zalevskaya, N. M., Russ.J.Org.Chem., CODEN: RJOCEQ, 32(4), <1996>, 524 - 529, Zh.Org.Khim., CODEN: ZORKAE, 32(4), <1996>, 545 - 550; BABS-6148286

RX

Reaction RID: 108026.30  
Reaction Classification: Chemical behaviour  
Reagent: O2, aq. sodium laurate  
Temperature: 75 Cel  
Pressure: 750.06 Torr  
Other Conditions: rate of emulsion oxidation; other sodium alkylcarboxylaates, var. organic solvents, var. pH  
Subject Studied: Mechanism  
Reference(s):  
1. Panicheva, L. P.; Turnaeva, E. A.; Panichev, S. A.; Yuffa, A. Ya., Pet.Chem.USSR (Engl.Transl.), CODEN: PECHAM, 38(3), <1998>, 164 - 169, Neftekhimiya, CODEN: NEFTAH, 338, <1998>, 179 - 184; BABS-6172166

RX

Reaction RID: 108026.31  
Reaction Classification: Preparation  
Reagent: NaCl, BaSO4, oxygen  
Note(s): Handbook  
Reference(s):  
1. Patent: Allied Chem. & Dye Corp. US 2776999 1952

RX

Reaction RID: 108026.32  
Reaction Classification: Preparation  
Reagent: aqueous NaOH, oxygen  
Note(s): Handbook  
Reference(s):  
1. Patent: Hercules Powder Co. US 2619510 1951  
2. Patent: Hercules Powder Co. US 2663740 1952  
3. Patent: Hercules Powder Co. US 2548435 1946  
4. Patent: Hercules Powder Co. US 2632772 1948  
5. Patent: Distillers Co. DE 926426 1949, DRP/DRBP Org.Chem.

RX

Reaction RID: 108026.33  
Reaction Classification: Preparation  
Reagent: aqueous NaOH, ozone, oxygen  
Note(s): Handbook  
Reference(s):  
1. Patent: Bergwerksges. Hibernia US 2827493 1952

RX

Reaction RID: 108026.34  
Reaction Classification: Preparation  
Reagent: NaHCO3, oxygen  
Note(s): Handbook  
Reference(s):  
1. Patent: Allied Chem. & Dye Corp. US 2577768 1949

RX

Reaction RID: 108026.35  
Reaction Classification: Preparation  
Reagent: Ca(OH)2, oxygen  
Note(s): Handbook  
Reference(s):  
1. Patent: Hercules Powder Co. US 2632774 1949

RX

Reaction RID: 108026.36  
Reaction Classification: Preparation

Reagent: CaCO<sub>3</sub>, oxygen  
Note(s): Handbook  
Reference(s):  
1. Patent: Allied Chem. & Cye Corp. US 2613227 1950  
2. Patent: Allied Chem. & Cye Corp. DE 864398 1951

Reaction:

RX

Reaction ID: 51759  
Reactant BRN: 1236613, 1098229  
Reactant: isopropylbenzene, methanol  
Product BRN: 1908117  
Product: 1-methyl-1-phenyl-ethyl hydroperoxide  
No. of Reaction Details: 1

Reaction Details:

RX

Reaction RID: 51759.1  
Reaction Classification: Preparation  
Reagent: oxygen  
Note(s): Handbook  
Reference(s):  
1. Patent: Montecatini US 2843633 1954

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FILE COVERS 1907 - 6 Sep 2002 VOL 137 ISS 11  
FILE LAST UPDATED: 5 Sep 2002 (20020905/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

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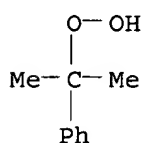
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      1940644 WATER
      212526 WATERS
      1991299 WATER
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      918320 H2O
      147657 AQUEOUS
            1 AQUEOUSES
      147658 AQUEOUS
            (AQUEOUS OR AQUEOUSES)
      926014 AQ
            118 AQS
      926086 AQ
            (AQ OR AQS)
      961992 AQUEOUS
            (AQUEOUS OR AQ)
L4      819 L3 AND (WATER OR H2O OR AQUEOUS)
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      1323492 MIXT
      458147 MIXTS
      1620917 MIXT
            (MIXT OR MIXTS)
      1667750 MIXTURE
            (MIXTURE OR MIXT)
      592411 COMPOSITION
      239065 COMPOSITIONS
      827686 COMPOSITION
            (COMPOSITION OR COMPOSITIONS)
      1164582 COMPN
      456556 COMPNS
      1419992 COMPN
            (COMPN OR COMPNS)
      1853040 COMPOSITION
            (COMPOSITION OR COMPN)
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L11 18 L1

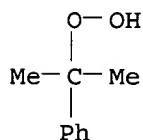
=> d ide

L11 ANSWER 1 OF 18 CHEMCATS COPYRIGHT 2002 ACS  
Accession No. (AN): 2002:1282035 CHEMCATS  
Catalog Name (CO): Acros Organics  
Publication Date (PD): 16 Apr 2002  
Order Number (ON): 34996  
Chemical Name (CN): Cumyl hydroperoxide  
Synonym (CN): Cumolhydroperoxid; Cumene hydroperoxide;  
Isopropylbenzolhydroperoxid;  
Isopropylbenzolhydroperoxid; Cumene hydroperoxide  
CAS Registry No. (RN): 80-15-9  
Structure :



=> d all

L11 ANSWER 1 OF 18 CHEMCATS COPYRIGHT 2002 ACS  
Accession No. (AN): 2002:1282035 CHEMCATS  
Catalog Name (CO): Acros Organics  
Publication Date (PD): 16 Apr 2002  
Order Number (ON): 34996  
Chemical Name (CN): Cumyl hydroperoxide  
Synonym (CN): Cumolhydroperoxid; Cumene hydroperoxide;  
Isopropylbenzolhydroperoxid;  
Isopropylbenzolhydroperoxid; Cumene hydroperoxide  
CAS Registry No. (RN): 80-15-9  
Purity : 80%  
Structure :



#### PROPERTIES

Density : 1.06  
Melting Point : -30 C  
Flash Point : 83.00

#### REGULATORY INVENTORIES

TSCA : Y  
EINECS : 201-254-7

#### REFERENCES

RTECS : MX2450000

#### PRICES

Quantity : 5.00 G, Price: \$8.90  
Quantity : 250.00 G, Price: \$27.00

#### COMPANY INFORMATION

Acros Organics  
Janssens Pharmaceuticaaan 3A  
Geel, 2440  
Belgium

Phone: +32 14 57 52 11  
Fax: +32 14 59 34 34  
Web: <http://www.acros.be>  
Email: [info@acros.com](mailto:info@acros.com)

FISHER SCIENTIFIC USA  
2000 Park Lane Drive  
Pittsburgh, PA, 15275-1126  
USA

Tel.: 1-800-766-7000  
Telefax: 1-800-926-1166

FISHER SCIENTIFIC  
1 Reagent Lane  
Fair Lawn, NJ, 07410  
USA

Tel.: 1-201.703.3163  
Fax: 1-201.703.3105

RESCO TRADE  
Hoveniersstraat 34 A  
Kortrijk, 8500  
Belgium

Tel.: +32 56 260 260  
Telefax: +32 56 260 270  
Telex: 85204 rtrade  
Filter Service NV/SA  
Handelsstrasse 16,  
4700 Eupen Belgium  
Tel.: +32 87 59 51 70  
Telefax: +32 87 59 51 79

KEM-en-TEC A/S  
Lers Parkall 42  
Copenhagen, DK-2100  
Denmark

Tel.: (\*\*45)39 27 17 77  
Fax: (\*\*45)39 20 01 78

UNITED SCIENTIFIC EQUIPMENT CO.  
49, Demeschk Street  
El-Mohandessin, Giza  
Egypt

Tel.: (\*\*20)2.361.4216  
Fax: (\*\*20)2.361.3211

BIO-ART  
Pepleri St. 12-23  
Tartu, EE-2400  
Estonia

Tel.: 003727434067  
Fax: 003727434067

TAMRO CORPORATION  
P O BOX 11  
Rajatorpantie 41B  
Fin, Vantaa, 01641  
Finland

Tel.: +358204454711  
Fax: +35804454717

ADVANCED TECHNOLOGY & INDUSTRIAL CO.  
8/F, Blk H, Kingland Building  
739 Nathan Road  
Mongkog, Kowloon  
Hong-Kong  
People's Republic of China

Tel.: (\*\*852)2390.2293  
Fax: (\*\*852)2789.8314

NEBOTRADE  
1394 Budapest  
Pf.: 360  
Budapest  
Hungary

Tel.: \*\*361 214 5000  
Fax: \*\*361 214 5000

ACCESSION NUMBER: 1977:600365 CAPLUS  
DOCUMENT NUMBER: 87:200365  
TITLE: Study of intermolecular interactions in the  
**cumene hydroperoxide-water**  
system by the proton magnetic resonance method  
AUTHOR(S): Markaryan, Sh. A.; Beileryan, N. M.; Grigoryan, S. K.  
CORPORATE SOURCE: Erevan. Gos. Univ., Yerevan, USSR  
SOURCE: Zh. Fiz. Khim. (1977), 51(9), 2385-7  
CODEN: ZFKHA9  
DOCUMENT TYPE: Journal  
LANGUAGE: Russian  
AB NMR data indicated that in the title system proton exchange occurs between  
PhCMe<sub>2</sub>OOH (I) and H<sub>2</sub>O. At 97:3 I-H<sub>2</sub>O the rate const. for this exchange is  
85 s<sup>-1</sup>. Interactions between the .pi. system of I and H<sub>2</sub>O also occur.  
IT Protonation and Proton transfer reaction  
(in **cumene hydroperoxide-water** system)  
IT Nuclear magnetic resonance  
(proton exchange in **cumene hydroperoxide-**  
**water** system in relation to)  
IT 7732-18-5, properties  
RL: PRP (Properties)  
(interaction of, with cumene hydroperoxide)  
IT 80-15-9  
RL: PRP (Properties)  
(interaction of, with water)

ACCESSION NUMBER: 1977:600365 CAPLUS  
DOCUMENT NUMBER: 87:200365  
TITLE: Study of intermolecular interactions in the  
**cumene hydroperoxide-water**  
system by the proton magnetic resonance method  
AUTHOR(S): Markaryan, Sh. A.; Beileryan, N. M.; Grigoryan, S. K.  
CORPORATE SOURCE: Erevan. Gos. Univ., Yerevan, USSR  
SOURCE: Zh. Fiz. Khim. (1977), 51(9), 2385-7  
CODEN: ZFKHA9  
DOCUMENT TYPE: Journal  
LANGUAGE: Russian  
AB NMR data indicated that in the title system proton exchange occurs between  
PhCMe2OOH (I) and H2O. At 97:3 I-H2O the rate const. for this exchange is  
85 s<sup>-1</sup>. Interactions between the .pi. system of I and H2O also occur.  
IT Protonation and Proton transfer reaction  
(in **cumene hydroperoxide-water** system)  
IT Nuclear magnetic resonance  
(proton exchange in **cumene hydroperoxide-**  
**water** system in relation to)  
IT 7732-18-5, properties  
RL: PRP (Properties)  
(interaction of, with cumene hydroperoxide)  
IT 80-15-9  
RL: PRP (Properties)  
(interaction of, with water)



```
=> s 15 and 1%
      7227471 1%
      (1)
L6      256 L5 AND 1%

=> s 15 and weight percent
      87980 WEIGHT
      7556 WEIGHTS
      93412 WEIGHT
      (WEIGHT OR WEIGHTS)
      1272798 WT
      94569 WTS
      1321675 WT
      (WT OR WTS)
      1348263 WEIGHT
      (WEIGHT OR WT)
      67936 PERCENT
      1270 PERCENTS
      69001 PERCENT
      (PERCENT OR PERCENTS)
      2940 WEIGHT PERCENT
      (WEIGHT(W) PERCENT)
L7      0 L5 AND WEIGHT PERCENT
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=> s 15 and percent water
      67936 PERCENT
      1270 PERCENTS
      69001 PERCENT
      (PERCENT OR PERCENTS)
      1940644 WATER
      212526 WATERS
      1991299 WATER
      (WATER OR WATERS)
      233 PERCENT WATER
      (PERCENT(W) WATER)
L8      0 L5 AND PERCENT WATER
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=> s 15 and % water
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      1991299 % WATER
      (WATER OR WATERS)
L9      209 L5 AND % WATER
```

```
=> d 200-209 ibib abs
```

```
L9  ANSWER 200 OF 209  CAPLUS  COPYRIGHT 2002 ACS
ACCESSION NUMBER:      1968:22368  CAPLUS
DOCUMENT NUMBER:       68:22368
TITLE:                  Copolymer of vinyl acetate and acrylamide
INVENTOR(S):            Lanthier, Raymond
PATENT ASSIGNEE(S):     Shawinigan Chemicals Ltd.
SOURCE:                 Brit., 10 pp.
                        CODEN: BRXXAA
DOCUMENT TYPE:          Patent
LANGUAGE:               English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:
```

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
GB 1092030		19671122		
PRIORITY APPLN. INFO.:		CA	19651015	
AB A process for prepg. aq. emulsions of a random copolymer of				

vinyl acetate (I) and acrylamide (II) contg. 6-15% II is described. Specific proportions of the monomers are copolymd. in an **aq.** medium with a redox catalyst system at a suitable pH (5-7) in a suitable temp. range (40-5.degree.) and with addn. of the ingredients to the polymn. medium in a manner that precluded undesired homopolymn. of either monomer. Thus, 30 g. I contg. 0.5 ml. tert-BuOOH (III) was added to a **mixt.** of **water** 250, II 10, and Gafac PE-510 (a polyoxyethylenated phosphate anionic surfactant) 1 g. The **mixt.** was agitated while a stream of N was introduced and heated to 40.degree.. Three solns. of 2 g. NaHSO3 and 2 g. Na2HPO4 in 50 ml. **H2O**, 30 g. II in 70 ml. **water**, and 1.5 ml. III in 348 g. I were added simultaneously over a period of 3 hrs. After cooling to room temp. and filtering through a stainless steel screen having 0.25-mm. openings, a smooth, creamy, stable emulsion contg. 54.02% solids was obtained. The I-II copolymer contained 10.6% II by wt. of the I in the copolymer. It had superior strength when used as an adhesive to bond 2 blocks of hardwood.

L9 ANSWER 201 OF 209 CAPLUS COPYRIGHT 2002 ACS  
 ACCESSION NUMBER: 1967:517526 CAPLUS  
 DOCUMENT NUMBER: 67:117526  
 TITLE: Dienic monomer polymerization using alcohol-peroxide catalysts system  
 INVENTOR(S): Burke, Oliver W., Jr.; Stahly, Eldon E.  
 SOURCE: U.S., 4 pp.  
 CODEN: USXXAM  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 3333015		19670725	US	19631119

AB Unsatd. liquid polymers of C4-8 conjugated diene monomers for use in the formation of protective coatings, inks, and adhesives are prepd. in the presence of an org. peroxy free radical generating catalyst in homogeneous **mixt.** with a C1-6 alc. Thus, butadiene 70.5, methacrylic acid 4.5, iso-PrOH 35.0, and 75% cumene hydroperoxide 4.0 parts was heated to 130.degree. while being stirred at 600 rpm. and maintained for 1.5 hrs., 25 parts styrene added, the polymn. continued for 1.5 hrs. at 130.degree., and the **mixt.** devolatilized at 140.degree./<5 mm. to give a 57% yield of **water**-white polymer having Brookfield viscosity 4230 poises at 30.degree. and <0.2% volatiles. Other catalysts used were tert-butyl hydroperoxide, di-tert-butyl peroxide, p-menthane hydroperoxide, and partially peroxidized tung oil. tert-BuOH and MeOH could be used in place of iso-PrOH.

L9 ANSWER 202 OF 209 CAPLUS COPYRIGHT 2002 ACS  
 ACCESSION NUMBER: 1967:516810 CAPLUS  
 DOCUMENT NUMBER: 67:116810  
 TITLE: Color-stabilized epoxides  
 INVENTOR(S): Goldsmith, William F.; Marples, David F.  
 PATENT ASSIGNEE(S): Union Carbide Corp.  
 SOURCE: Brit., 8 pp.  
 CODEN: BRXXAA  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
GB 1074003		19670628	GB	19640624

AB Color-stabilized epoxides contain an inhibiting amt. of a peroxide **compn.**, which is added at 70-100.degree.C., and are used to prep. color-stabilized resins. Thus, 5 wt. % 30% **aq.** H2O2 was added to 1000 g. 3,4-epoxy-6-methylcyclohexylmethyl 3,4-epoxy-6-methylcyclohexanecarboxylate, the **mixt.** heated at 95-7.degree.C. for 3 hrs., and the **water** evapd. to 70-80.degree.C./1 mm. for 2 hrs. to give an epoxy compd. having Gardner color 5.5 after 1 hr. at 350.degree.F. compared to 11.5 for an unstabilized epoxide. Varying the amt. of 30% **aq.** H2O2 affected the color stability after 16 hrs. at 98 +/- 2.degree. as follows (wt. % 30% **aq.** H2O2 and Gardner color given): 0, 5.7; 0.1, 1.2; 0.3, 1.2; 1.0, 1.2; 3.0, 3.0; 10.0, 7.0. Org. peroxides were similarly used as stabilizers.

L9 ANSWER 203 OF 209 CAPLUS COPYRIGHT 2002 ACS  
ACCESSION NUMBER: 1967:491513 CAPLUS  
DOCUMENT NUMBER: 67:91513  
TITLE: Synthetic rubbers  
INVENTOR(S): Richter, Johannes; Herte, Paul; Bochmann, Dieter; Neupert, Hans  
SOURCE: Ger. (East), 4 pp.  
CODEN: GEXXA8  
DOCUMENT TYPE: Patent  
LANGUAGE: German  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DD 55827		19670505	DD	19660826

AB Synthetic rubbers with better overall properties are prepd. from 1,3-dienes such as butadiene (I) and its **mixt.** with styrene (II), acrylonitrile, or other vinyl homologs in the presence of special alkylaryl hydroperoxide catalysts. Thus, a typical **compn.** consists of I 70, II 30, resin acid 2.25, fatty acid 2.10, Wotamol 0.10, KOH 1.18, p-diisopropylbenzene monohydroperoxide (III) 0.18, triethylenetetramine 0.02, Na3PO4 0.10, and **water** 150 parts. Comparison of the above **compn.** with controls not using III showed that the test **compn.** had much better vulcanization values and lower Huggins const. Other hydroperoxide catalysts used were isopropylbenzene hydroperoxide and chlorotriisopropylbenzene monohydroperoxide.

L9 ANSWER 204 OF 209 CAPLUS COPYRIGHT 2002 ACS  
ACCESSION NUMBER: 1967:436225 CAPLUS  
DOCUMENT NUMBER: 67:36225  
TITLE: Polarographic analysis of waste **waters** from phenol and acetone production  
AUTHOR(S): Shleina, T. T.; Buzlanova, M. M.  
SOURCE: Zavod. Lab. (1967), 33(3), 290-3  
CODEN: ZVDLAU  
DOCUMENT TYPE: Journal  
LANGUAGE: Russian

AB The **mixt.** of acetophenone and mesityl oxide was reduced polarographically in 0.5N KOH medium at potentials E1/2 = -1.44 v. and E1/2 = -1.54 v. vs. Hg pool. The differential polarography and the addn. method for quant. evaluation were used. The other components of waste **waters** did not interfere. The relative error was +/- .4%. The **mixt.** of cumene hydroperoxide, H2O2, and acetophenone was reduced in 0.05N LiCl medium at potentials E1/2 = -0.3 v., E1/2 = -1.25 v., and E1/2 = -1.75 v. For quant. evaluation the calibration curves of single standard components were used, with relative error +/- .2-4%. The sensitivity was 0.01-0.09 mg./ml. The detn. of .alpha.-methylstyrene (I) was made by the Alekseeva, et al., method (Alekseeva, et al., CA 59: 5341a) after conversion of I to the pseudo-nitroso compd. which was

reduced at potential  $E_{1/2} = 0.2$  v. compared with the S.C.E. The presence of PhOH >0.05 mg./ml. interfered. The relative error was  $\pm 0.3\%$ , the sensitivity 0.03 mg.I/ml.

L9 ANSWER 205 OF 209 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1967:422479 CAPLUS

DOCUMENT NUMBER: 67:22479

TITLE: Unsaturated polyester curing system consisting of cumene hydroperoxide, methyl ethyl ketone peroxide, and thioglycolic acid

INVENTOR(S): Montesano, Lewis

PATENT ASSIGNEE(S): Bell Telephone Laboratories, Inc.

SOURCE: U.S., 2 pp.

CODEN: USXXAM

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 3318974		19670509	US	19650323

AB Styrene-polyester (I) is cured with a critical **mixt.** of free-radical initiators. Thus, 100 parts I, viscosity 600-750 cp., sp. gr. 1.11-1.13, a 7:3 **mixt.** of a polyester from phthalic anhydride, maleic anhydride, and propylene glycol with styrene, was thoroughly mixed with cumene hydroperoxide 0.25, Me Et ketone peroxide 0.5, and thioglycolic acid (II) 0.5 part. After 5 min. at room temp. the **mixt.** had gelled to form a **water**-white hard resin without cracks. The same results were obtained with 0.25 parts II.

L9 ANSWER 206 OF 209 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1967:116617 CAPLUS

DOCUMENT NUMBER: 66:116617

TITLE: Polyacrylonitrile solutions for spinning

PATENT ASSIGNEE(S): Farbenfabriken Bayer A.-G.

SOURCE: Neth. Appl., 12 pp.

CODEN: NAXXAN

DOCUMENT TYPE: Patent

LANGUAGE: Dutch

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
NL 6608595		19661227		

PRIORITY APPLN. INFO.: DE 19650623

AB Acrylonitrile, alone or with another ethylenic unsatd. monomer, in HCONMe<sub>2</sub> is polymd. at 30-60.degree. in the presence of an org. peroxide and an .alpha.-hydroxy-.alpha.-aminosulfone having the formula [RSO<sub>2</sub>C(R<sub>1</sub>)R<sub>2</sub>]<sub>n</sub>X, in which R is an aliphatic or aromatic hydrocarbon radical, R<sub>1</sub> and R<sub>2</sub> are H atoms or alkyl radicals, n is 1 or 2, and X is OH or NR<sub>3</sub>, R<sub>3</sub> being an alkyl, hydroxyalkyl or an aryl radical, optionally with addn. of a strong mineral acid. Thus, in a closed 100-ml. app. completely filled, the reaction **mixt.** consisted of 65 g. HCONMe<sub>2</sub>, 32.7 g. acrylonitrile, and 2.3 g. Me acrylate. The polymerization took place in the presence of 0.3 g. cumene hydroperoxide and 0.3 g. (ClC<sub>6</sub>H<sub>4</sub>SO<sub>2</sub>CH<sub>2</sub>)<sub>2</sub>NMe. The filled app. was kept at 45.degree. for 10 hrs. in a **water** bath. The relative viscosity of 0.5% polymer soln. at 20.degree. in HCONMe<sub>2</sub> was 1.85, yield was 59%, and the soln. was pale yellow. With 0.2 g. concd. H<sub>2</sub>SO<sub>4</sub> in addn. to the above ingredients, the yield was 51%, relative viscosity 1.94, and the soln. was colorless.

L9 ANSWER 207 OF 209 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1967:37567 CAPLUS  
DOCUMENT NUMBER: 66:37567  
TITLE: Oxidation of sulfoxides with hydroperoxides  
AUTHOR(S): Kuhnén, Ludwig  
CORPORATE SOURCE: Chem. Werke Huels A.-G., Marl, Ger.  
SOURCE: Angew. Chem. (1966), 78(20), 937  
CODEN: ANCEAD

DOCUMENT TYPE: Journal

LANGUAGE: German

AB Sulfides and sulfoxides were oxidized to sulfones by equimolar amts. of org. hydroperoxides in the presence of V, Mo, or Ti compds. in almost quant. yields. The sulfides and sulfoxides, dissolved in benzene, EtOAc, or EtOH, were mixed with the catalyst and heated to 50 to 70.degree., and the org. hydroperoxide was then added slowly. The reaction was complete as soon as only traces of peroxide could be detected with KI in the reaction **mixt.** The sulfones were then isolated by crystn. or distn. PhSMe in benzene was oxidized with tert-butyl hydroperoxide in the presence of molybdenyl acetylacetonate to produce PhSO<sub>2</sub>Me in 98% yield. Me<sub>2</sub>SO<sub>4</sub> was oxidized with cumyl .alpha.-hydroperoxide in the presence of V<sub>2</sub>O<sub>5</sub> to give Me<sub>2</sub>SO<sub>2</sub> in 91% yield. These reactions proceeded without the presence or formation of **water** or carboxylic acids.

L9 ANSWER 208 OF 209 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1967:19053 CAPLUS  
DOCUMENT NUMBER: 66:19053  
TITLE: Vinyl chloride polymers or copolymers  
PATENT ASSIGNEE(S): Societa Edison S.p.A.-Settore Chimico  
SOURCE: Neth. Appl., 11 pp.  
CODEN: NAXXAN

DOCUMENT TYPE: Patent

LANGUAGE: Dutch

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
NL 6601847		19660823		

PRIORITY APPLN. INFO.: IT 19650222

AB The polymerization or copolymerization of vinyl chloride at low temps. and in the presence of a tetravalent Ce salt and an organometallic compd. of Ge, Sn or Pb as catalyst is terminated at a desired degree of conversion of the monomer by addn. of a peroxide, e.g. H<sub>2</sub>O<sub>2</sub>, cumyl hydroperoxide, cyclohexanone peroxide, or tert-Bu hydroperoxide, which are supplied in an amt. of 0.001-5 parts by wt. per 100 parts by wt. of monomer. The pH of the reaction **mixt.** is brought to <4 after addn. of the peroxide. A perfectly white polymer is obtained and discoloration by the presence of traces of the Ce salt is prevented. The polymer has a high crystallinity, a syndiotactic index of 2-2.8, and a mol. wt. of 20,000-200,000, and is suitable for the prepn. of fibers, films, and tubes resistant to boiling **water** and chlorinated solvents. For example, a **mixt.** of 500 g. anhyd. vinyl chloride, 3.2 ml. Et<sub>4</sub>Pb, and a soln. of 0.9 g. cerium ammonium nitrate in 120 ml. MeOH was polymerized in a N atm. at -40.degree.. After 2 hrs. and 45 min., a soln. of 0.4 ml. 35% H<sub>2</sub>O<sub>2</sub> and 0.3 ml. concd. HNO<sub>3</sub> in 30 ml. MeOH was supplied and the polymerization stopped immediately. When H<sub>2</sub>O<sub>2</sub> was added, no after-polymerization took place.

L9 ANSWER 209 OF 209 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1967:18894 CAPLUS  
DOCUMENT NUMBER: 66:18894  
TITLE: Copolymerization of vinyl chloride and ethylene initiated by trialkylboron-peroxide catalyst systems  
AUTHOR(S): Misono, Akira; Uchida, Yasuzo  
CORPORATE SOURCE: Univ. Tokyo, Tokyo, Japan

SOURCE: Bull. Chem. Soc. Jpn. (1966), 39(11), 2458-63  
 CODEN: BCSJA8  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 AB Low-pressure copolymerization of vinyl chloride and ethylene is initiated by trialkylboronperoxide catalyst systems in a 1:1 **water**-MeOH **mixt.** at 0.degree.. In the presence of cocatalysts hydroperoxide, Et3P and Bu3B are active, while Ph3B is not. As cocatalysts, hydroperoxides, such as tert-BuOOH and cumene hydroperoxide, are more active than disubstituted peroxides such as Bz2O2, tert-BuOOB, and tert-Bu2O2, and azobis(isobutyronitrile). The highest catalytic activity is observed when the cocatalyst/catalyst mole ratio is 0.4. The initiating radical is suggested to be the hydroxy radical, and the initiating mechanism is discussed. The yield and the reduced sp. viscosity of the copolymer decrease rapidly with an increase in the ethylene content of the monomer **mixt.** The monomer reactivity ratios are: .gamma.1 (vinyl chloride) = 4.16 and .gamma.2 (ethylene) = 0.05. The copolymerization proceeds via a normal radical mechanism. The resulting copolymer shows characteristic ir absorption at .nu. 750 cm. -1 and N.M.R. at 8.37 .tau..

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(FILE 'HOME' ENTERED AT 14:39:42 ON 06 SEP 2002)

L1 FILE 'CAPLUS' ENTERED AT 14:40:04 ON 06 SEP 2002  
 3 S FREEZING POINT DEPRESSION (3W) LIQUID

L2 FILE 'BEILSTEIN' ENTERED AT 14:41:56 ON 06 SEP 2002  
 2 S CUMENE HYDROPEROXIDE/CN

FILE 'CAPLUS' ENTERED AT 14:45:59 ON 06 SEP 2002

L3 FILE 'REGISTRY' ENTERED AT 14:46:08 ON 06 SEP 2002  
 1 S CUMENE HYDROPEROXIDE/CN

FILE 'CAPLUS' ENTERED AT 14:46:33 ON 06 SEP 2002

L4 819 S L3 AND (WATER OR H2O OR AQUEOUS)

L5 375 S L4 AND (MIXTURE OR COMPOSITION)

L6 256 S L5 AND 1%

L7 0 S L5 AND WEIGHT PERCENT

L8 0 S L5 AND PERCENT WATER

L9 209 S L5 AND % WATER

=> s l9 and cumene/ti

2000 CUMENE/TI

22 CUMENES/TI

2022 CUMENE/TI

((CUMENE OR CUMENES)/TI)

L10 16 L9 AND CUMENE/TI

=> d ibib abs 1-16

L10 ANSWER 1 OF 16 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 2002:429321 CAPLUS

DOCUMENT NUMBER: 136:403494

TITLE: Process for separating phenol from a **mixture** comprising at least hydroxyacetone, **cumene**, **water** and phenol

INVENTOR(S): Schwarz, Christoph; Weber, Mark; Tanger, Uwe; Korte, Hermann-Josef; Ullrich, Jochen

PATENT ASSIGNEE(S): Phenolchemie G.m.b.H. & Co. K.-G., Germany

SOURCE: U.S. Pat. Appl. Publ., 9 pp.

CODEN: USXXCO  
DOCUMENT TYPE: Patent  
LANGUAGE: English  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2002066661	A1	20020606	US 2001-970856	20011005
WO 2002046133	A1	20020613	WO 2001-EP14029	20011130
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				

PRIORITY APPLN. INFO.: DE 2000-10060505 A 20001206

AB Phenol is sepd. from a **mixt.** contg. hydroxyacetone, cumene, H<sub>2</sub>O and phenol, by fractionating the **mixt.** in a process with a fractional distn. step and a phase sepn. step to provide a single phenol fraction contg. <300 ppm of hydroxyacetone. In the work-up by distn. of cleavage product **mixts.**, the hydroxyacetone can be removed from the cleavage product **mixt.** together with a phenol fraction from which the hydroxyacetone has to be removed. A process can be used for purifying cleavage product **mixts.** obtained in the cleavage of alkylaryl hydroperoxides such as cumene hydroperoxide. The process allows sepn. of phenol and acetone from **mixts.** obtained in the cleavage of cumene hydroperoxide.

L10 ANSWER 2 OF 16 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 2002:256835 CAPLUS  
DOCUMENT NUMBER: 136:296542  
TITLE: Decomposition of **cumene** oxidation product  
INVENTOR(S): Hertzog, Richard R.; Sifniades, Stylianos; Fisher, William Bernard  
PATENT ASSIGNEE(S): USA  
SOURCE: U.S. Pat. Appl. Publ., 8 pp., Cont. of U.S. Ser. No. 601,879.  
CODEN: USXXCO  
DOCUMENT TYPE: Patent  
LANGUAGE: English  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2002040165	A1	20020404	US 2001-865190	20010723
PRIORITY APPLN. INFO.:				
			US 1989-297333	B1 19890117
			US 1992-920811	B1 19920724
			US 1994-203845	B1 19940228
			US 1994-333929	B1 19941103
			US 1996-601879	A1 19960215

AB A process for decomp. a cumene oxidn. product **mixt.** contg. cumene hydroperoxide (CHP) and dimethylphenyl carbinol (DMPC) to produce phenol, acetone and alpha-Me styrene (AMS) with enhanced safety of operation and reduced byproduct formation comprises the steps: (a) mixing the cumene oxidn. product in a stirred or back-mixed reactor with an acid catalyst, with 10-100 % acetone relative to the amt. of acetone produced during the decompn. reaction, and with up to 4% addnl. amts. of **water** relative to the reaction **mixt.**, at an av. temp. between about 50-90.degree. for a time sufficient to lower the av. CHP

concn. of the reactor to 0.2-3.0%, and wherein a portion of DMPC is converted to dicumyl peroxide (DCP); then (b) reacting the reaction **mixt.** from step (a) at a temp. between about 120-150.degree. under plug-flow conditions for a time sufficient to decomp. substantially all residual CHP and at least 90% of the DCP formed in step (a).

L10 ANSWER 3 OF 16 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 2001:785348 CAPLUS  
DOCUMENT NUMBER: 135:305480  
TITLE: **Cumene** hydroperoxide production process  
INVENTOR(S): Zakoshanskii, V. M.; Gryaznov, A. K.; Vasil'eva, I. I.  
PATENT ASSIGNEE(S): Russia  
SOURCE: Russ., No pp. given  
CODEN: RUXXE7  
DOCUMENT TYPE: Patent  
LANGUAGE: Russian  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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RU 2146670	C1	20000320	RU 1998-108236	19980429
AB	Emulsion-free two-stage air oxidn. of cumene in absence of initiators, catalysts, additives, and alkali agents in at least two reactor system is described. In the first reactor, cumene conversion at temp. up to 111-95.degree. is maintained at the level of at least 16%. Process is carried out in countercurrent reactor using pure alkali-free cumene. Oxidn. products from the first-stage are treated with ammonium hydroxide soln. until pH at least 8 is reached. When two or more second-stage reactors are available, oxidn. products are treated in each subsequent rector of the system. Conversion of cumene in the second oxidn. stage is maintained at up to 25 wt % at temp. at least 100-85 C, oxidn. charge and oxidizing agent being supplied concurrently. In all first- and second-stage reactors, pressure is maintained at least 4 atm and molar ratio of supplied oxygen to maximally consumed oxygen is maintained within a range of 1.12-1.30. Oxidn. products from the last second-stage oxidn. reactor are distd. to give industrial-grade (63-93%) cumene hydroperoxide. Excessive cumene is returned into process to be treated with <b>aq.</b> ammonium soln. to pH 9-10. Recycle cumene from hydrogenation stage and fresh cumene are treated with <b>mixt.</b> of 5-10% <b>aq.</b> NaOH soln. and 5-10-% <b>aq.</b> sodium carbonate soln. Combined streams of the above-mentioned cumenes are washed with <b>water</b> at cumene-to- <b>water</b> ratio 1: (0.15-0.20). Concn. of cumene hydroperoxide in product rises with rate 2.5 to 4.5% per h, while selectivity is not below 94 mol % and cumene conversion 21-22 mol %.			

L10 ANSWER 4 OF 16 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 2001:45962 CAPLUS  
DOCUMENT NUMBER: 134:86026  
TITLE: Isopropylation process and zeolite catalysts for the manufacture of **cumene** from benzene and isopropanol or propylene and isopropanol  
INVENTOR(S): Cappellazzo, Oscar; Girotti, Gianni; Pollastri, Massimiliano; Lombardini, Sergio; Piccininno, Domenico  
PATENT ASSIGNEE(S): Enichem S.p.A., Italy  
SOURCE: Eur. Pat. Appl., 29 pp.  
CODEN: EPXXDW  
DOCUMENT TYPE: Patent  
LANGUAGE: English  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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DOCUMENT TYPE: Patent  
LANGUAGE: Polish  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
	PL 152006	B1	19901031	PL 1987-266435	19870625
AB	Shaking impure Me <sub>2</sub> CO obtained along with phenol in the acid decompn. of cumene hydroperoxide with 5-15% addnl. <b>water</b> and withdrawing the upper hydrocarbon layer gave Me <sub>2</sub> CO contg. <30% <b>water</b> , useful for the title process. Thus, a <b>mixt.</b> contg. Me <sub>2</sub> CO 69.23, phenol 0.33, mesityl oxide (I) 0.006, cumene 0.22, .alpha.-methylstyrene (II) 4.55, acetophenone (III) 0.01, and <b>water</b> 19.65% was shaken 30 s with 5% addnl. <b>water</b> , and after 15 min aging, a lower layer contg. Me <sub>2</sub> CO 74.18, phenol 0.01, I 0.003, cumene 0.8, II 0.5, III 0.007, and <b>water</b> 24.5% formed.				

L10 ANSWER 7 OF 16 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1990:514518 CAPLUS

DOCUMENT NUMBER: 113:114518

TITLE: Kinetic characteristics of decomposition of **cumene** hydroperoxide in solutions of perchloric acid in **water**-alcohol solvents

AUTHOR(S): Vinnik, M. I.; Kislina, I. S.; Bushmakin, L. G.

CORPORATE SOURCE: Inst. Khim. Fiz. im. Semenova, Moscow, USSR

SOURCE: Kinet. Katal. (1990), 31(3), 528-34

CODEN: KNKTA4; ISSN: 0453-8811

DOCUMENT TYPE: Journal

LANGUAGE: Russian

AB PhCMe<sub>2</sub>OOH (I) hydrolysis to PhCMe<sub>2</sub>OH and H<sub>2</sub>O<sub>2</sub> and its decompn. to PhOH and Me<sub>4</sub>CO were studied in HClO<sub>4</sub>-contg. ROH-**H<sub>2</sub>O** (R = Et, Pr, Me<sub>3</sub>C) **mixts.** The yield of PhOH and Me<sub>2</sub>CO decreased with increasing HClO<sub>4</sub> concn. PhOH and Me<sub>2</sub>CO were formed by 2 paths, 1 involving a I complex with H<sub>3</sub>O<sup>+</sup> ClO<sub>4</sub><sup>-</sup>.**H<sub>2</sub>O** and the other a I-H<sub>5</sub>O<sub>2</sub><sup>+</sup> complex.

L10 ANSWER 8 OF 16 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1990:157487 CAPLUS

DOCUMENT NUMBER: 112:157487

TITLE: Kinetics of **cumene** hydroperoxide decomposition in **aqueous** solutions with catalysis by perchloric acid and hydrochloric acid-alkali metal chloride **mixtures**

AUTHOR(S): Kislina, I. S.; Bushmakin, L. G.; Sysoeva, S. G.; Antonovskii, V. L.; Zakoshanskii, V. M.; Vinnik, M. I.

CORPORATE SOURCE: Inst. Khim. Fiz., Moscow, USSR

SOURCE: Kinet. Katal. (1989), 30(1), 229-32

CODEN: KNKTA4; ISSN: 0453-8811

DOCUMENT TYPE: Journal

LANGUAGE: Russian

AB Two mechanisms for the title process were found. In the first, the rate const. is proportional to the deriv. of the thermodyn. activities of acid and **water** and is identical for K<sup>+</sup>, Na<sup>+</sup>, and Li<sup>+</sup> solns. In the second, the rate const. is proportional to the concn. of H<sub>5</sub>O<sub>2</sub><sup>+</sup>.

L10 ANSWER 9 OF 16 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1987:120376 CAPLUS

DOCUMENT NUMBER: 106:120376

TITLE: Method of .alpha.-methylstyrene isolation from byproducts arising during phenol production by the **cumene** process

INVENTOR(S): Koval, Jan; Mikula, Oldrich; Revus, Milos; Komorova, Hana; Brezula, Ludovit; Stefanik, Ivan; Tatransky, Ivan; Krizka, Pavel; Danilla, Frantisek; Suva, Jan

PATENT ASSIGNEE(S): Czech.  
 SOURCE: Czech., 5 pp.  
 CODEN: CZXXA9  
 DOCUMENT TYPE: Patent  
 LANGUAGE: Slovak  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
	CS 234827	B1	19850416	CS 1983-4241	19830613
AB	Increasing the <b>water</b> content of a <b>mixt.</b> of the title byproducts (aliph. and arom. ketones, alcs., and heterocyclics) from the usual 1.5 to 14% enables sepn. of an azeotropic <b>mixt.</b> of Me <sub>2</sub> CO, PhCMe:CH <sub>2</sub> (I), cumene, <b>water</b> , and minor amts. of PhOH and PhCOMe at the column head, and crude PhOH discharge at the base. The head product is distd. in a second column with added NaOH, Me <sub>2</sub> CO is sepd. at the head, and PhONa is removed from the <b>aq.</b> phase. The org. phase is fractionated in a third column at 6-19 kPa and reflux ratio 10 to give pure cumene which is recycled into the oxidn. process, and a mixed cumene-I fraction which is hydrogenated. The reflux ratio is then changed to 6 to yield pure (>98%) I and distn. bottoms contg. dimers of I and PhCOMe which are collected and worked up sep.				

L10 ANSWER 10 OF 16 CAPLUS COPYRIGHT 2002 ACS  
 ACCESSION NUMBER: 1975:7928 CAPLUS  
 DOCUMENT NUMBER: 82:7928  
 TITLE: Catalytic activity of some silica-alumina-  
**water** (n SiO<sub>2</sub>.m Al<sub>2</sub>O<sub>3</sub>.xH<sub>2</sub>O) systems on the decomposition reaction of **cumene** hydroperoxide. IV. Infrared study of synthetic systems of aluminosilicates  
 AUTHOR(S): Cormos, Liviu; Popica, Stana  
 CORPORATE SOURCE: Rom.  
 SOURCE: Stud. Univ. Babes-Bolyai, Ser. Chem. (1974), 19(1), 19-24  
 CODEN: SUBCAB  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English

AB The ir spectrum of aluminosilicates was studied, in relation to their use as catalysts in decompn. of cumene hydroperoxide. Shifts of the ir bands in relation to **compn.** are given and correlated with the max. catalytic activity of aluminosilicates contg. 30% Al<sub>2</sub>O<sub>3</sub>. Mech. **mixts.** of Al<sub>2</sub>O<sub>3</sub> and SiO<sub>2</sub>, which are noncatalytic were also studied.

L10 ANSWER 11 OF 16 CAPLUS COPYRIGHT 2002 ACS  
 ACCESSION NUMBER: 1973:58042 CAPLUS  
 DOCUMENT NUMBER: 78:58042  
 TITLE: Removing sulfuric acid from **mixtures** arising from the acid fission of **cumene** hydroperoxide  
 INVENTOR(S): Boehme, Guenter; Kiessling, Wolfgang; Moll, Karl  
 Klaus; Raue, Bernd  
 SOURCE: Ger. (East), 4 pp.  
 CODEN: GEXXA8  
 DOCUMENT TYPE: Patent  
 LANGUAGE: German  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DD 91643		19720805	DD 1971-153765	19710315

AB The title process involves extn. with a small amt. of **water** and eliminates the need for neutralization of the **mixt.** and subsequent deposition of salts in distn. columns. Thus, a cumene hydroperoxide decompn. **mixt.** contg. cumene 0.80, PhCOMe 0.95, Me2PhCOH 0.05, **H2O** 0.60, Me2CO 34.90, .alpha.-methylstyrene (I) 1.10, PhOH 57.45, higher phenols 2.10, I dimer 0.60, phenol tar 1.20, mesityl oxide 0.15, and H2SO4 0.10 wt. % was treated countercurrently at 4 l./hr in an extn. column filled with Raschig rings with 1 l./hr **H2O** at 40.degree. (theor. step no. 0.24) to give a **mixt.** contg. <10 mg/l. H2SO4. Eight further examples illustrated changes in extn. conditions.

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ACCESSION NUMBER: 1970:445113 CAPLUS  
DOCUMENT NUMBER: 73:45113  
TITLE: Removal of salts from phenol and acetone obtained by decomposition of **cumene** hydroperoxide  
INVENTOR(S): Janda, Jan; Koval, Jan; Kukel, Jan  
SOURCE: Czech., 3 pp.  
CODEN: CZXXA9  
DOCUMENT TYPE: Patent  
LANGUAGE: Czech  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
CS 131559		19690315	CS	19670209

AB Requisite conditions are described which reduce the content of inorg. salts in the org. phase <0.01% and prevent clogging of the boiler and column. Thus, a **mixt.**, after acid hydrolysis of cumene hydroperoxide, contg. 3 kg AcH, 2656 kg Me2CO, 55 kg mesityl oxide, 56.2 kg cumene, 215.3 kg PhCMe:CH2, 3935.6 kg PhOH, 41.5 kg PhCOMe, 115.2 kg cumenylphenol, 14.7 kg Me2CPhOH, 357.8 kg pitch, 5.6 kg H2SO4, and 50.5 kg **H2O**, was homogenized at 55.degree. with a soln. prepd. from PhONa and phenol **water**, contg. 203.5 kg PhONa, 402.7 kg PhOH, 14.9 kg Me2CO, 3.7 kg PhCOMe, 5.6 kg p-cumylphenol, and 1545.5 kg **H2O**. The **mixt.** was treated at 55.degree. with 85.3 kg 94% H2SO4 to give 2 layers in 30 min. The upper org. layer contained all org. substances, 12% **H2O**, and 0.008% Na2SO4, while the lower **aq.** layer contained 25% Na2SO4, 0.3% PhOH, and 0.6% Me2CO. The content of Na3SO4 in the org. phase dropped to 8% and the Na salts of org. acids passed into the **aq.** layer.

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ACCESSION NUMBER: 1970:78664 CAPLUS  
DOCUMENT NUMBER: 72:78664  
TITLE: Continuous catalytic cleavage of **cumene** hydroperoxide with sulfuric acid  
INVENTOR(S): Mantegazz, Attilio; Reni, Cesare  
PATENT ASSIGNEE(S): Societa Italiana Resine S.p.A.  
SOURCE: Ger., 5 pp.  
CODEN: GWXXAW  
DOCUMENT TYPE: Patent  
LANGUAGE: German  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 1443329		19700102		

PRIORITY APPLN. INFO.: IT 19620110

AB Cumene hydroperoxide (I) is converted to phenol (II) and acetone (III) by homogeneous catalytic cleavage with H2SO4 in a heat-exchanger to remove

the reaction heat. Thus, 500 parts of a previous cleavage **mixt.** is recycled with a pump to a velocity of 2 .times. 105 parts/hr. The heat-exchanger is fed with **H2O** at 90.degree. until the recycled **mixt.** reaches 70.degree., then it is cooled with **water** at 25.degree.. I (81.9% in cumene) 1000 parts/hr and 98% H2SO4 2 parts/hr is added continuously to the recycled flow (ratio 1:217), while 1002 parts/hr reaction **mixt.** is removed continuously from the system. The concn. of I never exceeds 0.1% during the reaction, the temp. is kept at 70-2.degree. at normal pressures. The product **mixt.** is neutralized by ion-exchangers and the products are sepd. by distn. yielding 98% II and 96% III.

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ACCESSION NUMBER: 1968:410222 CAPLUS  
DOCUMENT NUMBER: 69:10222  
TITLE: Separation of **cumene** hydroperoxide decomposition products  
INVENTOR(S): Nixon, Joseph R., Jr.  
PATENT ASSIGNEE(S): Hercules Inc.  
SOURCE: U.S., 5 pp.  
CODEN: USXXAM  
DOCUMENT TYPE: Patent  
LANGUAGE: English  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 3365375	A	19680123	US 1965-448414	19650415

AB The products obtained by catalytic decompn. of cumene hydroperoxide are sepd. by distn. in a distn. tower divided into 2 zones of approx. equal size by a horizontal baffle plate. Substantially pure acetone contg. .ltoreq. 1% **water** is withdrawn from the head of the column, hydrocarbons and **water**, both free of acetone and phenol, are withdrawn from an intermediate point of the column, and phenol contg. small amts. of **water**, heavy ends, and hydrocarbons is withdrawn from the base of the column. The acetone and hydrocarbon fractions are suitable for use in subsequent operations without further purification. The distn. process is economical because only a single distn. tower is required. Thus, 100 parts/hr. of catalyst-free cumene hydroperoxide decompn. product comprising acetone 45.3, **water** 11.6, hydrocarbons 4.8, phenol 35.6, and heavy ends 2.7% is introduced at the midpoint of a distn. column contg. 55 plates and sepd. in the center by a baffle plate. Live steam is also introduced at 8.6 parts/hr. at the column midpoint, and high pressure steam is introduced at 67 parts/hr. to the base of the distn. column. The amt. of steam used was equiv. to 1944 Btu./lb. of acetone introduced and sepd. A ratio of 4 parts of reflux/part of distillate removed at the column head is employed. Acetone, contg. <1% **water**, is removed at 44.3 parts/hr. from the column head. A **mixt.** of hydrocarbons and **water** is recovered from the midpoint of the distn. column. The **mixt.** is sepd. by decantation, and 4.6 parts/hr. hydrocarbons and 16.9 parts/hr. **water** are recovered, while 46 parts/hr. hydrocarbons and 19.5 parts/hr. **water** are returned as reflux. A **mixt.** of phenol 86.2, **water** 6.8, hydrocarbons 0.5, and heavy ends 6.5% is recovered from the bottom of the distn. column at the rate of 41.3 parts/hr. The acetone product contained no traces of phenol and could be recycled for use in the catalytic decompn. of cumene hydroperoxide.

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ACCESSION NUMBER: 1968:108273 CAPLUS  
DOCUMENT NUMBER: 68:108273  
TITLE: Catalytic activity of nSiO2.mAl2O3.xH2O systems in the decomposition reaction of **cumene**

hydroperoxide. I  
AUTHOR(S): Pop, Augustin; Krobl, Paul; Cormos, Liviu; Lengyel, Gheorghina  
CORPORATE SOURCE: Univ. " Babes-Bolyai", Cluj, Rom  
SOURCE: Stud. Univ. Babes-Bolyai, [Ser.] Chem. (1967), 12(2), 89-95  
CODEN: SUBCAB  
DOCUMENT TYPE: Journal  
LANGUAGE: Russian

AB The systems  $n\text{SiO}_2.m\text{Al}_2\text{O}_3.x\text{H}_2\text{O}$  (where  $n = 0-20$ ,  $m = 0-5$ , and  $x = 0-3$  at 420 and 580.degree. activation temp.) were prepd. by copptg. the mixed gels in proportions desired, from a soln. contg. free silicic acid and  $\text{Al}(\text{NO}_3)_3$ , at room temp., adding gradually  $(\text{NH}_4)_2\text{CO}_3$  soln.; a voluminous gel formed at pH .apprx.5. The filtered ppt. is left to dry in free air for several days, is dried at 105.degree., is ground and classified, and is heat-treated. The **compn.** obtained ranged from 100%  $\text{SiO}_2$  to 100%  $\text{Al}_2\text{O}_3$ . D.T.A. and differential thermogravimetric anal. curves (10.degree./min., in air) showed that absorbed  $\text{H}_2\text{O}$  is removed at <350.degree., with max. rate at 130.degree., most of the **water** of crystn. is removed at <700.degree., with the max. rate at 460-70.degree., and the remainder is removed at <1000.degree. at a const. rate. No addnl. modifications were indicated at <550.degree., but at <550.degree. the establishment of chem. bonds between the 2 oxides were indicated, concomitant with elimination of the last amts. of  $\text{H}_2\text{O}$ . The optimal activation temps. were 420.degree. (where the **water** of crystn. removal was min.) and 580.degree. (where the **water** of crystn. removal became const.). The sp. surface decreased with increase of the  $\text{Al}_2\text{O}_3$  proportion from 423 m.<sup>2</sup>/g. at 0%  $\text{Al}_2\text{O}_3$ , to 291 m.<sup>2</sup>/g. at 84.9%  $\text{Al}_2\text{O}_3$ . The catalytic properties of the systems were studied by using cumene hydroperoxide (I) decompn. as a reaction model. The expts. were effected in a static-type glass reactor, with internal and external cooling (most perfect cooling is essential to remove the reaction heat under isothermal conditions). In each expt. 21 g. of a 10% I soln. was treated with 2.2 g. catalyst, at 20, 30, and 40.degree., agitating strongly. The unconverted I was detd. iodometrically. For the 2 systems with  $m = 4$ ,  $n = 1$  and with  $m = 2.5$ ,  $n = 1$ , the sp. reaction rate consts. were: at 20.degree. 0.093, 0.04; 30.degree. 0.21, 0.08; 40.degree. -0.37, 0.16; the resp. activation energy values were 12.5 and 12.4 kcal./mole. Examn. of the variation of the conversion as function of the system **compn.** and of the temp. of activation and of reaction, showed that max. conversion was obtained for the system with  $m = 3$ ,  $n = 1$ ; the conversion increased with both temps., obtaining 94% at 40.degree..

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ACCESSION NUMBER: 1967:422479 CAPLUS  
DOCUMENT NUMBER: 67:22479  
TITLE: Unsaturated polyester curing system consisting of **cumene** hydroperoxide, methyl ethyl ketone peroxide, and thioglycolic acid  
INVENTOR(S): Montesano, Lewis  
PATENT ASSIGNEE(S): Bell Telephone Laboratories, Inc.  
SOURCE: U.S., 2 pp.  
CODEN: USXXAM  
DOCUMENT TYPE: Patent  
LANGUAGE: English  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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US 3318974		19670509	US	19650323

AB Styrene-polyester (I) is cured with a critical **mixt.** of free-radical initiators. Thus, 100 parts I, viscosity 600-750 cp., sp. gr. 1.11-1.13, a 7:3 **mixt.** of a polyester from phthalic

anhydride, maleic anhydride, and propylene glycol with styrene, was thoroughly mixed with cumene hydroperoxide 0.25, Me Et ketone peroxide 0.5, and thioglycolic acid (II) 0.5 part. After 5 min. at room temp. the **mixt.** had gelled to form a **water**-white hard resin without cracks. The same results were obtained with 0.25 parts II.

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